

Binding of Telomestatin, TMPyP4, BSU6037 and BRACO19 to a Telomeric G-Quadruplex-Duplex Hybrid Probed by All-Atom Molecular Dynamics Simulations with Explicit Solvent

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Table S1. Ligand potency and selectivity values from literature.

G-quadruplex ligand	Affinity (10^6 M^{-1})	Selectivity ¹	TRAP-LIG EC ₅₀ (μM) ¹
Telomestatin	24°C (FRET-melting assay)	70	0.6
TMPyP4	20 ¹	2	8.9
BRACO19	30 ¹	10	6.3

1: Reference 42 in text (C. Hounsol, L. Guittat, D. Monchaud, M. Jourdan, N. Saettel, J. L. Mergny and M. P. Teulade-Fichou, *Chem. Med. Chem.*, 2007, 2, 655-666.).

Table S2. Oxygen to Potassium Distance. Values are reported in Å. Colors refer to G4 layer: top (red); middle (green); bottom (blue). Values in red represent outliers from the data trend.

Residue:Oxygen:Pottassium	Crystal (PDB)	Apo form Simulation	Telomestatin (Top binding)	TMPyP4 ¹ (Interface)	BSU6037 ¹ (Interface)	BRACO19 (Interface)
G1:O6:K1	2.72	2.27±0.13	2.72±0.12	2.82±0.12	2.70±0.15	2.71±0.12
G5:O6:K1	2.98	2.71±0.13	2.71±0.12	2.68±0.13	2.76±0.17	2.72±0.14
G9:O6:K1	2.69	2.73±0.14	2.70±0.12	2.67±0.11	2.73±0.14	2.71±0.14
G14:O6:K1	2.76	2.71±0.14	2.70±0.14	2.74±0.14	2.71±0.14	2.72±0.13
G2:O6:K1	2.63	2.83±0.18	2.85±0.22	2.55±0.21	2.91±0.28	2.87±0.20
G6:O6:K1	2.74	2.86±0.20	2.92±0.23	3.15±0.18	2.85±0.22	2.82±0.19
G10:O6:K1	2.65	2.82±0.18	2.87±0.20	3.01±0.17	2.93±0.24	2.91±0.25
G15:O6:K1	2.74	2.90±0.24	2.99±0.28	2.98±0.34	2.88±0.26	2.82±0.20
G2:O6:K2	2.85	2.97±0.26	2.91±0.17	2.79±0.21	2.89±0.22	2.88±0.21
G6:O6:K2	3.18	2.89±0.20	2.89±0.22	2.76±0.23	2.90±0.25	2.92±0.23
G10:O6:K2	2.89	2.88±0.22	2.86±0.20	2.68±0.15	2.91±0.23	2.85±0.18
G15:O6:K2	3.26	2.91±0.23	2.91±0.22	2.89±0.20	2.92±0.27	2.89±0.21
G3:O6:K2	2.66	2.69±0.13	2.71±0.12	2.63±0.12	2.72±0.13	2.70±0.12
G9:O6:K2	2.66	2.73±0.14	2.72±0.13	2.50±0.12	2.72±0.14	2.73±0.14
G11:O6:K2	2.63	2.71±0.13	2.75±0.14	2.80±0.18	2.74±0.15	2.76±0.15
G16:O6:K2	2.64	2.71±0.13	2.72±0.15	2.79±0.15	2.72±0.14	2.75±0.15

¹ Mean values reported for this system were calculated with consideration to the portion of the simulation where the K⁺ cation was bound inside of the G-quadruplex structure.

Table S3. Oxygen to Oxygen Distance. Values are reported in Å. Colors refer to G4 layer: top (red); middle (green); bottom (blue).

Residue:Oxygen- Residue:Oxygen	Crystal (5dww)	Apo form Simulation	Telomestatin (Top binding)	TMPyP4 (Interface)	BSU6037 (Interface)	BRACO19 (Interface)
G1:O6-G5:O6	2.99	3.34±0.22	3.42±0.25	3.33±0.21	3.39±0.19	3.39±0.22
G5:O6-G9:O6	3.08	3.34±0.22	3.38±0.22	3.37±0.14	3.34±0.23	3.39±0.23
G9:O6-G14:O6	2.97	3.35±0.24	3.47±0.23	3.41±0.24	3.40±0.20	3.40±0.26
G14:O6-G1:O6	2.97	3.35±0.22	3.39±0.23	3.44±0.18	3.44±0.23	3.42±0.24
G2:O6-G6:O6	3.12	3.06±0.17	3.05±0.16	2.99±0.14	3.01±0.18	3.02±0.17
G6:O6-G10:O6	3.00	3.02±0.16	3.05±0.15	2.95±0.20	3.07±0.16	3.02±0.18
G10:O6-G15:O6	3.02	3.04±0.16	3.08±0.18	3.01±0.20	3.00±0.18	3.02±0.18
G15:O6-G2:O6	2.97	3.35±0.22	3.39±0.23	3.44±0.18	3.44±0.23	3.42±0.24
G3:O6-G7:O6	3.59	3.41±0.19	3.40±0.19	3.47±0.15	3.39±0.19	3.44±0.18
G7:O6-G11:O6	3.47	3.40±0.18	3.42±0.20	3.35±0.25	3.36±0.16	3.36±0.19
G1:O6-G16:O6	3.54	3.39±0.19	3.38±0.19	3.36±0.16	3.36±0.18	3.38±0.18
G16:O6-G3:O6	3.45	3.40±0.18	3.40±0.21	3.32±0.22	3.36±0.19	3.39±0.19
G1:O6-G2:O6	3.63	3.49±0.26	3.45±0.27	3.43±0.29	3.42±0.25	3.48±0.26
G5:O6-G6:O6	3.59	3.49±0.27	3.51±0.28	3.39±0.14	3.47±0.26	3.46±0.27
G9:O6-G10:O6	3.73	3.47±0.27	3.47±0.23	3.33±0.22	3.61±0.29	3.51±0.29
G14:O6-G15:O6	3.52	3.49±0.28	3.43±0.26	3.51±0.22	3.68±0.29	3.40±0.24
G2:O6-G3:O6	3.11	3.30±0.21	3.30±0.21	3.37±0.22	3.43±0.24	3.32±0.22
G6:O6-G7:O6	3.25	3.34±0.23	3.33±0.20	3.36±0.19	3.31±0.21	3.30±0.22
G10:O6-G11:O6	3.15	3.35±0.23	3.34±0.17	3.45±0.16	3.40±0.23	3.44±0.24
G15:O6-G16:O6	3.27	3.30±0.23	3.30±0.23	3.32±0.15	3.52±0.29	3.35±0.22

Table S4. DNA duplex structural parameters in different modes (abnormal values are in red) of the d(CGATCG)₂–drug system.

Base pair-Axis Parameters:

X-displacement (Å):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	-0.18	-1.18±1.49	-0.94±0.94	-2.18±1.09	-1.30±1.18	-1.49±0.76
2) C 21-G 29	-0.45	-1.36±0.93	-1.06±0.68	-2.15±1.01	-0.59±0.93	-1.04±0.72
3) G 22-C 28	0.26	-0.83±0.93	-0.09±0.61	-1.09±0.73	-0.39±0.93	-0.59±1.16
4) T 23-A 27	-0.92	-0.12±1.31	-0.42±0.73	-0.08±1.52	0.51±0.69	-0.13±0.67
5) T 24-A 26	-0.79	0.21±1.27	-0.52±1.01	-0.48±0.61	-0.19±2.08	0.57±1.08

Y-displacement (Å):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	0.60	0.25±0.88	1.17±0.87	0.94±0.66	0.63±1.08	0.75±0.74
2) C 21-G 29	0.34	0.12±1.18	1.32±0.77	0.86±0.73	0.36±0.97	0.79±0.79
3) G 22-C 28	0.18	0.77±0.87	1.22±0.74	1.19±0.85	0.47±0.74	1.13±0.55
4) T 23-A 27	0.43	-0.03±0.75	0.47±0.63	0.78±0.44	-0.19±0.75	0.64±0.70
5) T 24-A 26	0.36	-1.23±0.79	0.89±1.05	-0.68±0.52	-1.31±1.33	-1.31±1.11

Inclination (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	4.50	10.41±10.74	18.22±10.09	10.63±6.52	12.00±7.72	7.69±7.65
2) C 21-G 29	-3.1	10.65±12.25	14.80±8.65	13.06±11.02	18.28±13.46	12.31±5.69
3) G 22-C 28	5.10	14.40±12.97	12.37±11.22	14.79±13.40	12.94±15.09	13.12±5.15
4) T 23-A 27	3.00	3.16±17.20	10.79±9.89	9.50±18.53	-8.73±21.95	9.78±12.14
5) T 24-A 26	3.40	69.71±15.07	28.85±7.34	75.25±13.17	28.52±90.22	75.58±10.28

Tip (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	4.20	6.81±5.80	5.43±6.39	6.97±5.32	4.70±12.31	8.83±4.96
2) C 21-G 29	6.90	4.46±5.88	-2.55±6.12	0.22±4.91	-2.55±13.73	4.04±5.06
3) G 22-C 28	3.00	-0.57±6.55	-5.27±6.70	-3.33±4.80	-8.44±12.41	-0.68±4.89
4) T 23-A 27	-5.50	27.72±75.70	-9.56±6.46	-8.05±114.20	112.72±112.16	5.06±57.85
5) T 24-A 26	-0.80	47.69±34.18	-12.46±31.89	58.67±53.15	41.56±57.63	35.41±25.29

Axis Bend (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	---	---	---	---	---	---
2) C 21-G 29	0.40	2.65±0.98	2.93±1.10	3.15±0.69	5.42±1.75	3.26±0.93
3) G 22-C 28	0.40	2.01±0.75	2.24±0.87	2.39±0.53	4.36±1.53	2.50±0.77
4) T 23-A 27	0.40	1.99±0.74	2.24±0.87	2.37±0.55	4.47±1.69	2.50±0.77
5) T 24-A 26	0.60	2.59±0.98	2.91±1.13	3.09±0.73	5.97±2.25	3.25±1.02

Base pair-Step Parameters:**Shear (Å):**

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	0.26	-0.10±0.35	0.05±0.29	-0.04±0.24	0.02±0.28	-0.03±0.36
2) C 21-G 29	0.06	0.09±0.26	0.08±0.27	0.07±0.26	-0.09±0.26	-0.08±0.22
3) G 22-C 28	0.20	-0.05±0.31	-0.08±0.28	0.16±0.36	-0.04±0.30	-0.05±0.30
4) T 23-A 27	-0.43	0.04±0.37	-0.08±0.32	0.01±0.45	0.14±0.23	-0.09±0.28
5) T 24-A 26	-0.07	0.08±1.59	-0.58±1.87	-0.58±0.36	-2.78±5.89	-1.06±0.83

Stretch (Å):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	0.11	0.01±0.10	0.09±0.10	0.01±0.10	0.04±0.09	0.02±0.14
2) C 21-G 29	-0.03	-0.02±0.08	0.04±0.12	0.02±0.08	0.02±0.08	0.08±0.10
3) G 22-C 28	0.04	-0.03±0.07	0.03±0.10	-0.01±0.15	-0.01±0.14	0.07±0.09
4) T 23-A 27	0.08	0.03±0.13	0.05±0.20	0.01±0.07	0.08±0.15	0.06±0.13
5) T 24-A 26	0.32	-1.02±1.45	-4.35±1.87	-0.90±0.84	-0.31±87	-1.14±0.83

Stagger (Å):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	-0.50	-0.17±0.39	-0.49±0.47	-0.08±0.30	0.07±0.27	-0.27±0.35
2) C 21-G 29	0.47	0.01±0.26	0.06±0.20	0.26±0.36	-0.08±0.48	0.05±0.32
3) G 22-C 28	0.14	0.02±0.37	0.21±0.46	0.26±0.31	0.32±0.36	0.31±0.52
4) T 23-A 27	0.09	-0.01±0.50	-0.08±0.32	-0.08±0.27	0.36±0.46	-0.08±0.46
5) T 24-A 26	-0.23	-1.27±3.39	-3.29±0.43	-0.63±3.66	-3.14±0.99	-2.74±2.22

Buckle (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	-21.80	-13.16±10.19	-22.01±13.56	-9.79±4.36	-2.21±14.42	-13.79±7.29
2) C 21-G 29	1.10	-1.74±7.82	-5.96±7.73	-10.30±6.80	0.98±14.00	-2.29±9.21
3) G 22-C 28	-3.00	-5.32±9.79	1.52±9.51	-2.10±7.94	-3.90±9.08	3.98±11.65
4) T 23-A 27	-1.70	7.53±9.45	9.85±12.63	-3.22±10.13	-5.02±12.64	7.31±14.85
5) T 24-A 26	-4.20	-128.59±8.08	-31.61±44.95	-125.09±10.73	-26.16±46.08	-128.38±8.72

Propel (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	3.20	-3.66±5.50	-4.72±8.47	-15.94±4.30	-8.49±8.90	3.25±11.77
2) C 21-G 29	-9.60	-2.17±12.74	-2.97±10.94	-10.84±6.31	-12.55±7.47	-2.39±6.73
3) G 22-C 28	-7.20	-2.84±11.66	-4.21±8.82	-5.40±7.08	-2.28±10.11	-6.52±8.65
4) T 23-A 27	-38.40	-2.89±7.76	-2.17±10.37	-11.85±9.56	-1.98±5.06	-8.48±8.17
5) T 24-A 26	-33.60	-54.35±88.35	-13.69±34.31	-19.47±107.82	-6.93±38.97	-80.86±67.50

Opening(degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20-C 30	-1.00	1.79±1.86	3.29±3.38	1.61±2.47	1.71±2.91	-0.73±3.24
2) C 21-G 29	-0.60	0.69±1.84	1.07±2.55	1.11±3.57	2.31±4.84	0.39±2.74
3) G 22-C 28	1.60	-0.63±3.59	1.70±2.42	1.13±2.77	1.25±3.13	0.75±4.21
4) T 23-A 27	-10.20	6.67±5.66	1.62±6.06	3.58±5.22	3.15±5.30	3.49±7.63
5) T 24-A 26	-15.20	21.7±28.90	-6.49±31.41	-1.26±44.14	55.71±158.93	32.24±31.46

Paired Base-Base Parameters:**Shift(Å):**

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20/C 21	-0.62	-0.35±0.75	-0.76±0.90	-0.49±0.56	0.33±0.56	-0.02±0.36
2) C 21/G 22	0.25	0.09±0.68	0.31±0.68	0.46±0.37	-0.07±1.09	-0.19±0.68
3) G 22/T 23	-1.19	0.04±0.98	-0.35±0.59	-0.55±0.39	-0.27±0.98	0.13±0.67
4) T 23/T 24	0.02	0.62±1.31	0.55±1.45	1.06±1.53	-0.41±2.56	0.49±1.18

Slide (Å):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20/C 21	-0.28	-0.33±0.38	0.17±0.49	-0.95±0.56	-0.59±0.44	-0.39±0.44
2) C 21/G 22	-0.16	0.33±0.41	0.07±0.50	-0.14±0.37	0.27±0.36	0.30±0.91
3) G 22/T 23	0.24	-0.62±0.31	-0.39±0.42	-0.49±0.39	-0.40±0.35	-0.24±0.47
4) T 23/T 24	-0.54	0.53±1.90	1.58±0.35	-0.45±1.53	3.08±2.32	0.65±1.22

Rise (Å):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20/C 21	2.86	3.18±0.38	2.98±0.25	3.37±0.10	3.25±0.22	3.27±0.31
2) C 21/G 22	3.48	3.45±0.41	3.08±0.27	3.11±0.19	3.42±0.24	3.28±0.24
3) G 22/T 23	3.38	3.24±0.31	3.25±0.29	3.11±0.30	3.18±0.38	3.34±0.28
4) T 23/T 24	3.40	2.81±1.90	4.98±0.64	2.07±2.20	2.06±2.51	3.57±1.58

Tilt (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20/C 21	-9.00	-3.92±3.19	-6.40±5.73	-1.93±4.71	2.40±5.90	-1.41±3.72
2) C 21/G 22	5.10	0.78±3.86	-0.71±4.85	0.99±5.36	-4.07±7.74	-2.74±5.50
3) G 22/T 23	-0.90	-0.48±3.77	2.21±3.84	3.25±3.67	1.66±2.49	2.40±3.56
4) T 23/T 24	2.80	38.19±44.75	29.24±12.44	16.91±48.88	72.87±96.36	46.59±31.96

Roll (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20/C 21	3.20	1.38±5.30	2.12±3.01	-0.12±4.59	0.57±6.02	-1.17±6.37
2) C 21/G 22	-3.00	5.20±11.22	7.64±5.55	6.21±3.71	6.73±8.80	3.46±6.80
3) G 22/T 23	-6.00	-0.14±6.85	3.36±5.96	4.04±5.66	3.24±3.83	-3.14±5.05
4) T 23/T 24	6.00	41.19±64.79	12.29±21.85	9.20±76.13	33.18±113.92	53.43±45.74

Twist (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20/C 21	19.50	24.69±4.35	29.91±6.79	34.21±3.02	30.49±5.95	29.89±5.92
2) C 21/G 22	37.20	42.46±3.62	35.33±8.21	33.56±5.67	39.70±5.64	35.71±8.34
3) G 22/T 23	34.00	26.09±3.21	26.07±3.84	28.68±6.41	23.97±5.20	30.10±7.35
4) T 23/T 24	33.50	7.23±27.24	32.40±12.74	-7.20±31.86	8.38±23.97	8.14±20.87

H-rise (Å):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20/C 21	2.90	3.06±0.44	2.93±0.35	3.18±0.27	2.94±0.27	3.20±0.35
2) C 21/G 22	3.44	3.37±0.27	2.98±0.40	2.99±0.24	3.25±0.28	3.27±0.34
3) G 22/T 23	3.36	2.89±0.20	3.00±0.29	2.69±0.61	2.77±0.47	3.18±0.24
4) T 23/T 24	3.37	2.01±2.68	4.95±0.98	2.95±0.97	3.19±2.82	2.83±2.10

H-twist (degree):

Base-pair	Crystal Structure (5dww)	DNA only simulation	Telomestatin (Top binding)	TMPyP4 (interface binding)	BSU6037 (Interface binding)	BRACO19 (interface binding)
1) G 20/C 21	20.00	25.45±4.02	30.94±6.46	34.50±2.94	30.74±5.56	30.17±5.81
2) C 21/G 22	36.90	43.61±3.29	36.79±8.10	34.24±5.99	41.12±4.43	36.41±7.85
3) G 22/T 23	33.80	26.36±3.93	27.24±3.86	29.89±5.98	25.10±4.56	29.83±7.21
4) T 23/T 24	33.80	25.06±34.96	35.97±18.31	20.34±49.23	22.41±121.19	30.46±24.43

Table S5. Backbone Dihedral Angles. Red indicates residues that are a part of the G-quadruplex core. Orange indicates residues that are a part of the interface.

Residue 1 (G1)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal (5DWW)	N/A	N/A	50.4	117.9	205.4	275.8	193.9	126.1
DNA only	N/A	N/A	94.0 \pm 4.3	126.5 \pm 2.8	186.7 \pm 2.6	264.5 \pm 4.0	236.1 \pm 5.1	144.8 \pm 2.7
Simulation	N/A	N/A	81.8 \pm 13.7	126.8 \pm 2.4	188.8 \pm 3.0	265.8 \pm 9.5	233.4 \pm 2.0	141.7 \pm 8.3
Telomestatin (Top binding)	N/A	N/A	94.2 \pm 7.9	132.8 \pm 2.5	229.4 \pm 5.8	181.1 \pm 5.4	269.8 \pm 7.6	145.4 \pm 4.2
TMPyP4 (interface)	N/A	N/A	64.2 \pm 5.6	135.9 \pm 2.8	238.5 \pm 34.7	186.2 \pm 20.2	62.1 \pm 16.4	150.5 \pm 3.4
BSU6037 (interface)	N/A	N/A	96.0 \pm 7.4	126.6 \pm 1.8	191.8 \pm 10.6	252.0 \pm 11.9	243.1 \pm 4.5	141.5 \pm 1.7
BRACO19 (Interface)	N/A	N/A						

Residue 2 (G2)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	107.1	183.8	192.1	143.7	200.7	177.4	238.5	154.3
DNA only	273.3 \pm 19.1	177.4 \pm 1.9	69.1 \pm 18.4	124.5 \pm 2.1	191.0 \pm 6.9	246.5 \pm 7.1	240.0 \pm 1.9	136.8 \pm 4.7
Telomestatin	277.6 \pm 17.8	177.6 \pm 1.0	63.1 \pm 19.1	120.8 \pm 5.4	189.9 \pm 6.0	252.9 \pm 5.2	238.4 \pm 2.0	129.4 \pm 9.4
TMPyP4	243.7 \pm 29.0	166.3 \pm 7.5	81.0 \pm 20.1	144.6 \pm 1.9	172.2 \pm 0.5	267.9 \pm 2.6	260.5 \pm 2.7	187.0 \pm 4.2
BSU6037	265.7 \pm 14.7	165.4 \pm 3.7	59.8 \pm 8.8	137.3 \pm 2.4	186.6 \pm 16.9	252.5 \pm 16.9	248.6 \pm 4.8	165.9 \pm 6.7
BRACO19	274.3 \pm 9.7	172.0 \pm 4.4	67.8 \pm 9.4	124.3 \pm 2.3	192.6 \pm 2.0	250.2 \pm 5.3	240.2 \pm 1.6	137.4 \pm 3.0

Residue 3 (G3)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	47.6	72.9	39.0	109.5	286.0	76.0	245.6	117.5
DNA only	280.2 \pm 14.4	174.2 \pm 1.6	64.6 \pm 13.7	132.5 \pm 4.7	284.3 \pm 2.2	79.4 \pm 1.4	241.7 \pm 1.3	146.0 \pm 8.3
Telomestatin	292.7 \pm 3.0	173.7 \pm 3.2	53.5 \pm 1.2	134.0 \pm 1.3	283.7 \pm 1.8	79.3 \pm 1.4	241.6 \pm 2.6	146.6 \pm 1.9
TMPyP4	289.6 \pm 2.3	181.3 \pm 1.0	55.1 \pm 0.9	123.3 \pm 1.6	277.1 \pm 1.1	76.7 \pm 1.6	243.8 \pm 2.0	130.5 \pm 3.4
BSU6037	290.1 \pm 2.9	172.3 \pm 5.6	55.5 \pm 2.6	127.3 \pm 5.3	280.6 \pm 7.3	77.8 \pm 0.9	238.5 \pm 3.4	136.9 \pm 8.1
BRACO19	283.8 \pm 5.5	173.9 \pm 1.1	61.7 \pm 4.0	134.7 \pm 2.2	286.4 \pm 2.6	81.0 \pm 0.8	242.0 \pm 1.3	148.7 \pm 3.7

Residue 4 (T4)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	62.2	121.6	50.6	109.3	250.8	135.8	227.2	113.0
DNA only	68.2 \pm 2.2	173.0 \pm 0.7	54.2 \pm 0.5	138.2 \pm 1.0	216.5 \pm 2.0	137.0 \pm 3.0	238.3 \pm 0.7	156.0 \pm 2.6
Telomestatin	67.7 \pm 2.9	172.1 \pm 1.9	54.0 \pm 1.8	137.9 \pm 3.1	216.7 \pm 11.0	137.1 \pm 13.7	238.6 \pm 4.8	156.7 \pm 4.1
TMPyP4	70.7 \pm 1.6	172.6 \pm 1.0	56.9 \pm 4.0	140.6 \pm 3.3	247.3 \pm 3.8	96.2 \pm 4.0	237.0 \pm 11.7	159.0 \pm 5.8
BSU6037	68.9 \pm 3.4	169.8 \pm 0.4	52.3 \pm 0.4	141.0 \pm 2.0	237.1 \pm 7.6	109.6 \pm 6.5	239.7 \pm 3.6	160.5 \pm 4.2
BRACO19	67.4 \pm 2.0	174.1 \pm 0.8	56.0 \pm 0.8	138.8 \pm 0.7	216.0 \pm 4.1	137.8 \pm 6.3	235.7 \pm 6.3	156.8 \pm 1.3

Residue 5 (G5)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	93.0	179.4	65.4	131.1	207.5	287.8	196.6	140.5
DNA only	79.1 \pm 3.8	190.4 \pm 2.4	67.1 \pm 14.9	138.4 \pm 0.5	195.9 \pm 1.2	274.4 \pm 1.2	225.2 \pm 1.9	166.1 \pm 3.2
Telomestatin	74.6 \pm 3.2	191.0 \pm 7.1	61.7 \pm 9.2	140.3 \pm 1.3	194.6 \pm 2.8	274.0 \pm 3.2	223.5 \pm 3.2	172.7 \pm 3.4
TMPyP4	67.0 \pm 2.0	173.2 \pm 2.6	55.7 \pm 3.5	143.1 \pm 0.9	182.9 \pm 1.3	273.3 \pm 1.3	239.3 \pm 2.0	165.9 \pm 2.5
BSU6037	71.3 \pm 4.5	182.3 \pm 10.7	56.6 \pm 0.9	141.3 \pm 2.8	188.1 \pm 3.2	269.6 \pm 1.0	229.9 \pm 2.6	170.9 \pm 1.5
BRACO19	78.5 \pm 2.5	190.4 \pm 2.6	63.2 \pm 4.2	140.0 \pm 1.0	200.0 \pm 2.6	275.7 \pm 2.4	223.2 \pm 1.2	169.8 \pm 1.3

Residue 6 (G6)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	258.9	179.7	43.1	107.2	155.5	273.1	250.0	122.3
DNA only	276.2 \pm 4.1	175.8 \pm 1.5	56.6 \pm 4.0	122.3 \pm 2.7	198.8 \pm 9.2	242.4 \pm 12.6	240.3 \pm 2.6	131.2 \pm 2.5
Telomestatin	276.1 \pm 13.1	177.7 \pm 2.3	58.3 \pm 13.4	121.1 \pm 2.8	190.2 \pm 7.4	254.0 \pm 8.7	239.2 \pm 1.1	131.8 \pm 3.9
TMPyP4	289.1 \pm 1.1	174.9 \pm 4.0	54.8 \pm 3.7	99.3 \pm 2.4	190.8 \pm 1.5	270.5 \pm 5.2	214.8 \pm 2.8	94.7 \pm 3.3
BSU6037	287.6 \pm 1.5	179.2 \pm 2.1	52.0 \pm 0.8	120.2 \pm 3.2	191.6 \pm 6.6	254.9 \pm 11.2	234.9 \pm 3.0	129.2 \pm 2.7
BRACO19	275.3 \pm 1.8	175.0 \pm 0.5	53.3 \pm 4.1	125.3 \pm 2.8	207.8 \pm 4.7	229.6 \pm 9.9	246.0 \pm 3.7	133.6 \pm 2.2

Residue 7 (G7)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	292.9	189.7	56.0	103.8	57.1	272.0	234.5	110.8
DNA only	284.9 \pm 11.8	170.9 \pm 3.0	59.7 \pm 9.0	131.3 \pm 4.2	284.7 \pm 1.9	80.5 \pm 1.2	239.8 \pm 0.9	143.9 \pm 7.0
Telomestatin	290.0 \pm 0.8	174.6 \pm 3.7	54.5 \pm 0.6	128.3 \pm 2.8	282.6 \pm 1.2	79.2 \pm 0.9	241.2 \pm 1.4	139.8 \pm 5.4
TMPyP4	287.9 \pm 3.5	176.9 \pm 1.5	58.6 \pm 3.3	141.4 \pm 1.8	295.7 \pm 3.4	83.5 \pm 0.7	242.3 \pm 1.8	154.2 \pm 4.6
BSU6037	291.3 \pm 1.7	171.4 \pm 3.0	56.4 \pm 0.4	132.7 \pm 2.3	278.3 \pm 4.2	78.9 \pm 2.2	237.7 \pm 2.2	143.8 \pm 4.8
BRACO19	288.3 \pm 3.4	162.1 \pm 1.2	57.0 \pm 3.4	135.1 \pm 2.0	281.9 \pm 11.3	84.8 \pm 7.5	240.3 \pm 0.8	147.2 \pm 2.5

Residue 8 (T8)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	149.7	173.7	58.4	149.0	204.2	94.6	225.6	168.4
DNA only	69.5 \pm 3.2	173.3 \pm 0.5	55.8 \pm 3.0	137.1 \pm 1.5	213.4 \pm 11.3	135.3 \pm 3.2	235.6 \pm 1.8	154.5 \pm 0.9
Telomestatin	71.9 \pm 7.7	174.2 \pm 0.5	60.7 \pm 14.7	135.7 \pm 2.0	198.7 \pm 19.9	143.7 \pm 11.2	237.9 \pm 2.7	153.5 \pm 3.0
TMPyP4	64.0 \pm 1.9	173.0 \pm 2.4	57.3 \pm 3.1	141.4 \pm 1.4	223.4 \pm 8.1	145.1 \pm 6.8	237.4 \pm 2.8	159.0 \pm 4.3
BSU6037	69.8 \pm 7.0	171.9 \pm 1.3	54.4 \pm 6.9	139.0 \pm 1.0	246.4 \pm 10.1	108.4 \pm 6.5	237.1 \pm 1.3	155.6 \pm 0.9
BRACO19	70.5 \pm 5.1	174.0 \pm 0.7	57.0 \pm 1.0	139.9 \pm 1.1	225.6 \pm 7.0	130.8 \pm 10.7	239.2 \pm 2.5	157.8 \pm 2.4

Residue 9 (G9)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	96.9	193.9	66.1	127.4	194.6	264.4	230.0	137.0
DNA only	82.3 \pm 14.9	187.7 \pm 1.6	69.7 \pm 15.9	138.4 \pm 1.0	196.8 \pm 2.4	273.7 \pm 2.0	224.8 \pm 1.3	164.6 \pm 2.2
Telomestatin	99.9 \pm 44.8	187.2 \pm 5.0	90.2 \pm 52.4	137.8 \pm 4.4	196.6 \pm 1.6	273.7 \pm 1.6	221.6 \pm 1.8	164.6 \pm 7.8
TMPyP4	67.8 \pm 3.1	186.3 \pm 5.7	50.8 \pm 2.7	142.6 \pm 2.6	213.6 \pm 5.1	285.7 \pm 4.1	211.3 \pm 3.8	184.5 \pm 5.8
BSU6037	72.8 \pm 1.2	176.8 \pm 5.0	55.1 \pm 1.2	141.7 \pm 1.0	192.0 \pm 2.1	267.6 \pm 1.2	223.0 \pm 3.8	177.5 \pm 4.2
BRACO19	74.3 \pm 4.1	186.1 \pm 2.6	58.6 \pm 2.2	139.3 \pm 1.7	198.1 \pm 4.3	276.5 \pm 4.2	222.4 \pm 1.8	171.6 \pm 3.9

Residue 10 (G10)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	271.4	181.7	49.2	136.3	190.2	229.6	256.3	145.5
DNA only	279.8 \pm 1.9	176.7 \pm 1.8	52.4 \pm 2.0	125.0 \pm 2.0	201.7 \pm 1.8	240.8 \pm 4.4	243.4 \pm 1.7	133.2 \pm 3.0
Telomestatin	281.6 \pm 2.2	176.7 \pm 3.0	53.7 \pm 2.1	123.5 \pm 3.1	197.0 \pm 6.6	249.3 \pm 5.7	241.2 \pm 1.1	133.1 \pm 4.2
TMPyP4	270.4 \pm 1.9	169.1 \pm 2.4	47.5 \pm 1.4	131.7 \pm 0.7	269.6 \pm 4.4	168.2 \pm 6.2	259.3 \pm 1.5	139.4 \pm 2.6
BSU6037	289.2 \pm 0.4	177.3 \pm 1.6	54.5 \pm 1.1	121.5 \pm 3.1	187.2 \pm 1.4	267.1 \pm 2.4	230.0 \pm 1.8	131.4 \pm 4.3
BRACO19	280.2 \pm 4.2	176.4 \pm 2.2	50.4 \pm 1.4	125.2 \pm 3.2	202.6 \pm 9.3	238.4 \pm 15.5	242.3 \pm 6.5	134.0 \pm 2.7

Residue 11 (G11)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	293.8	165.9	56.7	145.7	206.1	100.3	246.6	156
DNA only	284.4 \pm 2.8	171.3 \pm 3.1	52.3 \pm 2.3	136.2 \pm 0.6	246.6 \pm 21.1	83.8 \pm 1.8	247.5 \pm 3.6	149.7 \pm 1.2
Telomestatin	280.4 \pm 0.3	177.6 \pm 4.1	51.1 \pm 2.5	136.9 \pm 1.6	240.0 \pm 13.3	95.7 \pm 4.7	253.3 \pm 0.7	151.9 \pm 2.5
TMPyP4	280.9 \pm 2.2	131.8 \pm 3.0	51.5 \pm 1.6	129.0 \pm 3.9	273.1 \pm 3.7	81.3 \pm 3.0	236.1 \pm 2.5	135.7 \pm 5.8
BSU6037	290.9 \pm 2.3	174.6 \pm 2.6	53.5 \pm 1.8	122.5 \pm 2.7	274.9 \pm 2.9	73.9 \pm 2.0	232.5 \pm 5.2	128.3 \pm 4.1
BRACO19	285.6 \pm 2.6	169.0 \pm 6.7	53.6 \pm 2.0	140.5 \pm 0.9	268.3 \pm 4.3	156.0 \pm 8.2	244.2 \pm 3.1	151.4 \pm 2.0

Residue 12 (T12)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	75.2	177.4	63.1	138.2	207.4	61.7	248.6	163.6
DNA only	84.2 \pm 6.1	192.5 \pm 5.8	85.7 \pm 28.1	129.9 \pm 6.1	217.6 \pm 31.0	234.5 \pm 30.8	245.4 \pm 5.1	140.5 \pm 7.4
Telomestatin	135.2 \pm 18.6	182.8 \pm 9.2	104.0 \pm 46.9	134.2 \pm 4.4	258.3 \pm 12.9	150.7 \pm 50.5	241.0 \pm 5.0	145.0 \pm 7.6
TMPyP4	69.3 \pm 6.0	177.3 \pm 9.2	74.2 \pm 32.6	123.8 \pm 2.1	205.0 \pm 6.4	194.7 \pm 19.0	247.2 \pm 4.9	131.0 \pm 5.1
BSU6037	72.5 \pm 1.8	186.7 \pm 2.3	179.9 \pm 1.4	129.0 \pm 2.3	257.0 \pm 7.2	242.3 \pm 19.8	66.3 \pm 1.7	135.4 \pm 2.0
BRACO19	290.2 \pm 1.4	180.8 \pm 2.5	58.4 \pm 0.8	127.6 \pm 6.1	252.5 \pm 4.6	105.6 \pm 16.0	231.2 \pm 4.8	137.8 \pm 11.1

Residue 13 (T13)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	254.5	179.6	54.9	129.2	179.9	263.4	236.6	140.5
DNA only	273.3 \pm 25.9	178.5 \pm 4.3	67.9 \pm 14.5	127.3 \pm 7.5	218.1 \pm 24.7	171.3 \pm 76.4	247.3 \pm 4.6	134.4 \pm 15.4
Telomestatin	250.1 \pm 23.4	183.2 \pm 3.6	77.4 \pm 15.5	135.0 \pm 3.2	198.4 \pm 1.3	267.3 \pm 3.2	261.0 \pm 3.1	148.1 \pm 6.7
TMPyP4	275.1 \pm 7.4	169.3 \pm 2.4	59.4 \pm 0.9	129.2 \pm 7.5	235.2 \pm 8.6	119.3 \pm 16.1	244.1 \pm 3.5	144.6 \pm 7.9
BSU6037	70.3 \pm 2.6	188.3 \pm 8.8	57.7 \pm 0.7	137.4 \pm 1.5	241.6 \pm 5.3	73.0 \pm 1.8	241.8 \pm 1.9	152.8 \pm 3.9
BRACO19	158.7 \pm 39.9	174.8 \pm 5.3	76.4 \pm 9.3	134.1 \pm 2.3	224.8 \pm 24.0	129.4 \pm 17.4	225.7 \pm 19.2	150.1 \pm 4.8

Residue 14 (G14)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	179.4	179.4	48.5	131.2	195.8	269.9	222.0	142.0
DNA only	182.5 \pm 65.3	182.1 \pm 0.4	176.1 \pm 70.6	140.3 \pm 6.8	184.2 \pm 4.3	253.9 \pm 12.8	250.7 \pm 7.6	163.6 \pm 10.6
Telomestatin	277.9 \pm 3.7	179.4 \pm 2.7	283.9 \pm 9.4	147.5 \pm 3.3	189.8 \pm 3.1	266.3 \pm 1.1	238.7 \pm 4.1	174.5 \pm 5.3
TMPyP4	103.8 \pm 37.2	186.1 \pm 15.1	123.8 \pm 86.8	125.1 \pm 6.7	241.4 \pm 24.8	192.4 \pm 26.8	58.8 \pm 3.2	135.7 \pm 10.6
BSU6037	74.1 \pm 6.4	182.8 \pm 6.6	65.9 \pm 22.6	113.3 \pm 13.7	192.5 \pm 13.2	228.1 \pm 33.0	262.8 \pm 3.5	122.9 \pm 21.5
BRACO19	92.8 \pm 16.7	185.1 \pm 3.6	92.7 \pm 23.3	125.1 \pm 2.2	189.7 \pm 16.4	241.8 \pm 27.5	216.1 \pm 6.0	140.0 \pm 5.5

Residue 15 (G15)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal								
5DWW	278.9	186.4	41.5	133.7	198.8	227.7	255.2	146.3
DNA only	271.7±14.3	173.3±5.6	69.1±13.7	119.1±2.4	187.2±2.0	259.9±2.9	237.9±1.9	130.5±4.7
Telomestatin	268.1±19.1	176.2±2.1	67.8±19.3	116.9±3.2	187.0±2.7	259.4±4.5	240.7±2.4	126.3±6.0
TMPyP4	282.6±4.4	164.8±5.7	55.4±2.3	141.0±1.4	173.2±2.9	269.4±2.8	254.8±2.1	176.7±4.7
BSU6037	270.4±16.6	137.9±38.8	95.2±57.9	123.1±14.3	205.8±5.5	245.9±24.6	229.7±27.2	129.9±20.0
BRACO19	242.0±22.7	170.0±5.4	57.3±7.7	126.5±5.7	239.2±15.0	197.1±18.7	255.8±6.0	132.1±5.3

Residue 16 (G16)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW								
	40.0	187.1	286.1	135.9	173.4	272.4	250.4	186.9
DNA only	280.6±4.9	176.9±1.9	61.1±6.0	120.5±2.7	193.7±5.2	254.5±10.8	240.9±4.0	130.6±3.3
Telomestatin	277.4±10.3	176.1±4.0	65.6±11.4	120.3±7.1	187.7±2.1	259.4±2.8	242.5±6.1	129.4±13.3
TMPyP4	295.1±1.7	176.1±3.3	57.0±2.5	101.6±1.0	181.0±4.2	266.6±4.0	230.7±1.6	103.9±1.6
BSU6037	282.7±4.2	174.1±6.5	52.0±4.1	135.7±3.2	184.6±3.8	264.7±11.6	247.9±1.4	154.0±6.3
BRACO19	274.3±1.5	156.3±7.4	56.2±3.1	121.1±3.7	188.7±1.2	260.9±4.6	239.8±1.6	132.9±7.6

Residue 17 (T17)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW								
	159.6	180.5	176.8	126.1	179.8	272.3	235.5	138.3
DNA only	292.2±0.3	165.9±4.3	57.9±2.3	133.4±0.9	183.5±8.5	264.1±11.6	253.7±2.1	147.1±3.0
Telomestatin	287.9±7.6	167.4±2.1	64.8±8.0	133.1±2.7	176.4±7.7	272.7±2.2	251.2±5.4	147.5±2.5
TMPyP4	297.2±1.2	172.1±2.3	58.3±1.9	132.0±0.8	175.4±1.1	273.9±1.1	251.0±1.3	145.9±0.5
BSU6037	268.1±31.9	170.2±2.6	82.0±30.1	122.4±5.8	207.0±25.9	232.3±41.1	241.5±2.3	130.1±9.6
BRACO19	291.2±1.6	170.4±1.0	55.9±1.0	129.5±2.4	175.4±2.3	272.2±0.6	249.9±2.6	141.4±2.9

Residue 18 (T18)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal								
5DWW	301.6	166.6	63.3	107.3	6.5	68.6	215.3	109.7
DNA only	276.5±15.8	158.7±24.7	87.1±21.3	138.1±4.4	267.4±19.1	159.2±23.5	233.1±8.4	147.6±6.9
Telomestatin	294.3±5.3	162.1±26.8	73.3±27.0	138.9±4.3	284.0±21.4	147.5±30.7	235.2±9.7	146.3±5.3
TMPyP4	300.0±1.7	168.5±3.9	64.7±2.0	130.2±2.1	288.8±1.3	140.8±1.9	239.4±1.9	136.8±2.1
BSU6037	287.3±11.0	176.4±2.6	52.8±2.1	124.5±11.4	198.5±5.0	267.2±7.1	235.9±4.7	134.1±21.5
BRACO19	293.2±3.0	171.8±14.4	65.7±16.7	133.1±3.2	281.2±8.1	134.2±14.5	232.3±5.7	140.3±5.0

Residue 19 (A19)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal								
5DWW	60.3	150.7	183.7	124.2	261.8	268.1	173.4	137.5
DNA only	269.6±24.8	185.7±6.0	269.3±15.9	147.5±2.6	254.4±3.9	265.8±4.4	200.2±1.4	173.8±4.3
Telomestatin	297.7±1.3	181.5±5.6	301.1±5.9	148.6±4.3	257.7±17.0	260.2±6.2	197.6±2.5	173.6±2.7
TMPyP4	293.6±4.8	155.6±2.1	298.7±9.5	142.0±2.1	222.8±0.9	288.7±1.4	225.1±1.4	150.9±1.0
BSU6037	285.3±1.5	171.7±1.0	52.1±1.7	135.9±2.4	216.1±10.9	212.9±12.4	261.4±2.4	150.2±6.1
BRACO19	269.6±16.8	177.9±1.3	254.9±13.3	147.2±2.6	258.8±2.3	265.1±2.2	197.3±2.3	168.4±4.8

Residue 20 (G20)

System	α	β	γ	δ	ϵ	ζ	χ	Pucker
Crystal 5DWW	295.2	177.2	47.0	136.2	173.5	274.8	258.5	205.5
DNA only	281.5 \pm 4.6	171.5 \pm 1.1	54.4 \pm 4.7	137.2 \pm 2.5	196.4 \pm 5.9	244.4 \pm 7.0	257.1 \pm 1.7	166.1 \pm 7.0
Telomestatin	259.3 \pm 43.5	168.4 \pm 8.7	79.0 \pm 52.0	137.6 \pm 3.7	192.9 \pm 10.0	245.8 \pm 12.8	260.0 \pm 0.8	168.1 \pm 6.7
TMPyP4	285.4 \pm 2.4	186.4 \pm 1.8	57.0 \pm 1.5	122.0 \pm 1.8	190.0 \pm 2.3	265.8 \pm 1.5	221.6 \pm 2.7	131.3 \pm 3.6
BSU6037	285.0 \pm 1.0	166.0 \pm 1.2	51.5 \pm 3.1	137.2 \pm 4.1	185.1 \pm 2.8	262.0 \pm 3.5	244.1 \pm 4.9	162.5 \pm 7.1
BRACO19	271.1 \pm 12.6	178.9 \pm 0.7	71.1 \pm 13.6	140.4 \pm 0.3	180.0 \pm 0.3	266.4 \pm 1.0	250.3 \pm 0.9	174.1 \pm 1.8

Residue 21 (C21)

System	α	β	γ	δ	ϵ	ζ	χ	Pucker
Crystal 5DWW	299.2	168.0	55.9	102.7	171.1	273.8	234.9	107.5
DNA only	290.0 \pm 0.7	167.3 \pm 2.0	52.7 \pm 0.5	130.1 \pm 1.2	210.3 \pm 4.4	227.0 \pm 5.6	249.4 \pm 0.8	140.2 \pm 1.6
Telomestatin	293.0 \pm 2.9	167.9 \pm 4.3	52.5 \pm 1.8	131.7 \pm 1.6	207.3 \pm 5.6	231.8 \pm 7.8	249.8 \pm 2.1	142.1 \pm 4.0
TMPyP4	287.7 \pm 2.6	183.4 \pm 3.9	53.5 \pm 1.2	125.4 \pm 1.3	187.1 \pm 3.7	267.7 \pm 4.1	239.4 \pm 0.4	138.1 \pm 2.9
BSU6037	290.2 \pm 2.5	175.4 \pm 1.6	55.9 \pm 4.2	130.1 \pm 3.2	199.6 \pm 13.1	247.3 \pm 13.6	248.2 \pm 2.8	142.6 \pm 6.5
BRACO19	290.8 \pm 1.6	176.3 \pm 1.6	54.9 \pm 1.1	128.6 \pm 1.9	203.1 \pm 3.0	235.2 \pm 3.3	247.8 \pm 2.0	138.7 \pm 3.6

Residue 22 (G22)

System	α	β	γ	δ	ϵ	ζ	χ	Pucker
Crystal 5DWW	301.3	176.5	57.5	136.2	200.5	174.2	247.7	149.9
DNA only	287.3 \pm 1.4	167.2 \pm 1.4	52.6 \pm 0.5	134.0 \pm 1.2	180.1 \pm 1.9	259.9 \pm 4.6	250.0 \pm 1.0	161.7 \pm 1.5
Telomestatin	287.9 \pm 2.3	170.5 \pm 3.6	49.7 \pm 3.4	130.1 \pm 4.5	190.4 \pm 2.4	260.4 \pm 4.5	248.5 \pm 2.6	154.4 \pm 8.0
TMPyP4	288.0 \pm 4.1	175.6 \pm 2.8	53.2 \pm 3.7	130.1 \pm 4.7	186.4 \pm 3.7	249.0 \pm 7.3	252.8 \pm 2.4	144.9 \pm 8.5
BSU6037	287.0 \pm 2.2	173.4 \pm 4.3	51.5 \pm 4.0	128.7 \pm 2.2	185.5 \pm 2.6	261.8 \pm 2.9	244.0 \pm 1.5	148.7 \pm 6.2
BRACO19	285.6 \pm 3.1	167.5 \pm 1.8	55.6 \pm 4.6	131.2 \pm 2.4	184.8 \pm 1.7	259.8 \pm 2.5	247.8 \pm 2.8	153.7 \pm 4.1

Residue 23 (T23)

System	α	β	γ	δ	ϵ	ζ	χ	Pucker
Crystal 5DWW	28.3	75.0	55.1	110.5	191.9	277.9	241.1	123.0
DNA only	289.9 \pm 3.9	172.5 \pm 1.6	59.5 \pm 2.8	121.1 \pm 1.6	183.6 \pm 3.8	263.8 \pm 7.3	241.8 \pm 1.4	130.8 \pm 3.2
Telomestatin	289.4 \pm 2.8	168.8 \pm 2.3	55.9 \pm 1.3	118.0 \pm 2.4	181.1 \pm 2.6	271.7 \pm 1.6	247.3 \pm 3.6	122.8 \pm 5.3
TMPyP4	294.2 \pm 1.6	170.5 \pm 1.7	58.3 \pm 1.2	126.9 \pm 4.5	178.3 \pm 1.4	267.1 \pm 2.5	246.8 \pm 4.0	142.5 \pm 6.8
BSU6037	287.0 \pm 8.1	176.0 \pm 2.0	59.8 \pm 7.9	136.4 \pm 1.2	184.3 \pm 2.6	276.5 \pm 2.6	254.5 \pm 2.1	149.8 \pm 3.5
BRACO19	292.8 \pm 0.6	172.3 \pm 1.5	57.6 \pm 0.5	122.7 \pm 0.7	182.1 \pm 1.3	266.5 \pm 1.0	243.3 \pm 0.6	134.1 \pm 0.8

Residue 24 (T24)

System	α	β	γ	δ	ϵ	ζ	χ	Pucker
Crystal 5DWW	285.1	165.6	56.2	105.4	164.1	277.7	249.1	116.2
DNA only	293.3 \pm 1.1	173.6 \pm 2.1	57.3 \pm 1.0	124.9 \pm 3.5	185.0 \pm 4.7	266.2 \pm 12.7	247.2 \pm 3.1	134.7 \pm 7.7
Telomestatin	290.7 \pm 2.1	171.5 \pm 1.7	56.8 \pm 1.4	110.7 \pm 7.3	202.1 \pm 10.7	246.3 \pm 32.8	249.5 \pm 5.1	108.7 \pm 13.3
TMPyP4	295.9 \pm 2.1	173.2 \pm 1.6	58.2 \pm 1.6	138.2 \pm 1.8	265.5 \pm 0.6	170.7 \pm 2.1	242.6 \pm 1.9	145.2 \pm 0.8
BSU6037	296.4 \pm 1.2	168.1 \pm 0.6	61.0 \pm 1.4	127.7 \pm 1.2	184.0 \pm 3.4	253.0 \pm 5.9	71.0 \pm 2.8	141.0 \pm 1.9
BRACO19	292.2 \pm 1.3	172.7 \pm 1.0	58.3 \pm 1.1	125.3 \pm 0.8	184.9 \pm 0.9	271.1 \pm 2.4	247.6 \pm 0.6	134.7 \pm 0.6

Residue 25 (A25)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	310.0	164.3	61.3	133.8	0.0	0.0	245.5	138.6
DNA only	284.6 \pm 13.8	173.0 \pm 2.9	57.8 \pm 2.3	118.2 \pm 6.1	0.0 \pm 0.0	0.0 \pm 0.0	175.4 \pm 86.8	127.5 \pm 10.9
Telomestatin	261.2 \pm 31.9	189.0 \pm 9.7	60.9 \pm 10.5	121.0 \pm 4.0	0.0 \pm 0.0	0.0 \pm 0.0	269.5 \pm 12.3	132.3 \pm 10.2
TMPyP4	279.6 \pm 1.3	70.3 \pm 0.9	175.8 \pm 0.9	113.2 \pm 5.3	0.0 \pm 0.0	0.0 \pm 0.0	56.2 \pm 2.2	110.3 \pm 7.8
BSU6037	289.1 \pm 1.4	174.1 \pm 1.5	56.5 \pm 0.9	130.7 \pm 4.7	0.0 \pm 0.0	0.0 \pm 0.0	242.2 \pm 5.1	156.1 \pm 11.0
BRACO19	288.4 \pm 3.3	174.1 \pm 0.5	55.5 \pm 1.0	122.5 \pm 0.8	0.0 \pm 0.0	0.0 \pm 0.0	243.6 \pm 1.3	134.1 \pm 3.3

Residue 26 (A2)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	N/A	N/A	192.2	149.8	175.1	271.6	249.4	189.3
DNA only	N/A	N/A	58.5 \pm 1.5	136.7 \pm 1.1	190.7 \pm 4.4	269.6 \pm 3.4	54.5 \pm 0.9	154.7 \pm 1.0
Telomestatin	N/A	N/A	57.7 \pm 2.1	141.8 \pm 3.5	242.0 \pm 23.2	109.9 \pm 83.7	50.6 \pm 2.6	158.6 \pm 3.7
TMPyP4	N/A	N/A	59.6 \pm 4.8	131.4 \pm 2.2	206.8 \pm 3.1	277.8 \pm 2.5	53.7 \pm 3.4	140.7 \pm 4.8
BSU6037	N/A	N/A	73.7 \pm 11.0	137.6 \pm 3.3	185.0 \pm 2.7	279.6 \pm 1.2	61.4 \pm 1.4	150.4 \pm 3.4
BRACO19	N/A	N/A	61.4 \pm 5.9	135.9 \pm 0.9	193.9 \pm 3.3	267.3 \pm 8.6	66.0 \pm 23.1	153.5 \pm 1.3

Residue 27 (A3)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	156.8	186.1	177.2	128.9	206.2	274.9	226.1	136.7
DNA only	288.0 \pm 0.7	170.8 \pm 0.2	54.4 \pm 0.7	129.9 \pm 0.6	197.0 \pm 1.0	239.1 \pm 1.1	264.9 \pm 1.5	145.5 \pm 1.1
Telomestatin	270.2 \pm 10.2	165.1 \pm 2.4	61.9 \pm 5.3	139.2 \pm 3.7	168.6 \pm 17.4	268.4 \pm 17.6	276.8 \pm 5.4	180.4 \pm 18.9
TMPyP4	285.2 \pm 3.0	174.1 \pm 1.4	53.3 \pm 1.2	133.6 \pm 1.4	183.3 \pm 1.9	257.7 \pm 3.4	271.6 \pm 1.0	156.9 \pm 4.9
BSU6037	295.2 \pm 2.5	170.5 \pm 2.4	63.1 \pm 1.3	136.0 \pm 2.7	170.3 \pm 4.3	272.5 \pm 2.5	265.5 \pm 2.1	172.5 \pm 3.8
BRACO19	287.9 \pm 1.3	170.5 \pm 0.7	53.1 \pm 0.5	130.2 \pm 1.6	198.6 \pm 2.4	241.4 \pm 5.1	264.7 \pm 2.4	144.9 \pm 3.4

Residue 28 (C4)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	285.8	160.2	58.2	135.4	198.0	165.1	256.2	143.5
DNA only	287.8 \pm 6.2	163.5 \pm 4.7	59.0 \pm 11.1	126.2 \pm 0.5	211.4 \pm 3.6	234.9 \pm 3.8	246.9 \pm 4.6	134.3 \pm 1.4
Telomestatin	291.8 \pm 1.3	174.2 \pm 6.9	55.8 \pm 1.6	130.2 \pm 4.9	225.2 \pm 7.7	210.8 \pm 15.0	254.0 \pm 7.5	137.3 \pm 5.6
TMPyP4	292.4 \pm 1.0	164.2 \pm 1.2	55.4 \pm 1.5	114.1 \pm 2.4	204.2 \pm 6.3	237.5 \pm 8.8	245.5 \pm 2.0	113.5 \pm 5.5
BSU6037	295.2 \pm 2.2	174.5 \pm 3.5	54.9 \pm 1.5	127.0 \pm 2.9	211.5 \pm 10.7	222.5 \pm 16.0	252.6 \pm 2.8	132.9 \pm 3.0
BRACO19	283.8 \pm 11.9	153.2 \pm 16.7	73.5 \pm 28.6	121.0 \pm 1.3	206.1 \pm 1.7	248.4 \pm 9.6	238.4 \pm 10.3	129.0 \pm 1.7

Residue 29 (G5)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	35.0	69.6	42.5	88.3	199.5	288.3	219.1	84.8
DNA only	282.7 \pm 4.0	170.9 \pm 1.3	52.7 \pm 2.2	135.7 \pm 0.7	196.1 \pm 1.9	262.0 \pm 3.0	255.9 \pm 2.6	161.3 \pm 3.0
Telomestatin	284.9 \pm 2.6	164.0 \pm 1.4	49.2 \pm 2.7	136.8 \pm 2.9	195.5 \pm 4.3	262.1 \pm 7.3	253.0 \pm 1.5	163.1 \pm 10.5
TMPyP4	286.9 \pm 2.7	169.1 \pm 3.0	55.3 \pm 2.0	137.9 \pm 2.8	177.7 \pm 3.8	266.5 \pm 4.9	252.7 \pm 2.3	165.6 \pm 4.0
BSU6037	286.8 \pm 4.5	164.9 \pm 3.9	52.2 \pm 2.0	138.7 \pm 2.4	185.2 \pm 4.7	257.8 \pm 4.1	250.3 \pm 2.1	166.9 \pm 4.8
BRACO19	284.5 \pm 1.2	171.1 \pm 1.6	52.5 \pm 0.3	133.8 \pm 0.7	195.2 \pm 2.0	249.8 \pm 3.2	252.8 \pm 2.1	155.8 \pm 2.1

Residue 30 (C6)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	283.8	169.4	58.1	129.7	281.9	165.0	267.7	134.5
DNA only	282.9±6.7	157.6±9.0	65.5±14.6	124.0±3.6	213.9±7.7	242.5±7.4	253.7±4.3	128.8±5.7
Telomestatin	283.7±1.0	165.9±1.3	55.9±1.9	119.5±5.5	207.5±9.6	248.2±7.6	256.5±2.7	121.8±14.3
TMPyP4	291.9±1.9	174.0±3.4	58.1±0.7	128.3±2.2	176.6±2.8	270.9±1.1	246.0±3.0	142.5±1.8
BSU6037	291.7±3.3	177.6±1.4	54.6±1.9	129.2±2.9	181.2±1.2	269.3±2.0	244.9±1.1	144.8±5.4
BRACO19	289.8±0.7	165.6±1.1	56.7±1.0	131.6±0.9	172.5±0.8	271.1±0.6	252.5±0.6	148.4±1.4

Residue 31 (T7)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	292.2	137.5	59.6	131.0	322.1	81.0	234.0	137.0
DNA only	200.4±36.4	170.1±8.5	167.7±37.9	141.6±2.2	296.3±13.1	96.4±12.5	242.0±3.6	154.3±4.7
Telomestatin	200.2±80.5	178.3±11.5	169.2±85.3	137.3±5.8	259.4±17.4	128.0±20.4	239.9±7.2	151.8±9.7
TMPyP4	297.3±1.6	172.2±2.7	62.1±1.7	120.1±0.9	196.3±3.6	272.6±2.2	235.8±2.6	129.5±2.6
BSU6037	290.5±3.7	172.9±4.0	58.2±5.7	119.0±2.9	194.1±7.8	258.0±8.0	241.2±1.5	123.0±4.5
BRACO19	295.0±0.4	179.6±0.3	56.9±0.7	119.1±0.6	187.6±0.1	274.5±0.5	234.8±0.9	128.0±0.8

Residue 32 (A8)

System	α	β	γ	δ	ε	ζ	χ	Pucker
Crystal 5DWW	61.8	193.0	183.2	110.3	0.0	0.0	162.3	110.4
DNA only	133.2±54.4	185.7±2.7	128.4±43.3	122.7±2.0	0.0±0.0	0.0±0.0	173.7±11.2	128.2±3.2
Telomestatin	219.5±9.1	180.0±3.0	57.8±6.8	121.5±3.3	0.0±0.0	0.0±0.0	184.6±2.9	127.0±6.8
TMPyP4	291.0±2.8	173.1±3.1	53.7±0.9	138.6±0.5	0.0±0.0	0.0±0.0	275.6±1.2	157.8±3.0
BSU6037	287.2±4.2	171.7±4.3	53.0±1.2	130.1±3.7	0.0±0.0	0.0±0.0	250.3±3.6	142.0±7.0
BRACO19	291.8±0.2	168.0±0.4	56.1±0.5	110.6±0.3	0.0±0.0	0.0±0.0	61.2±1.2	112.0±0.3

Table S6. DNA G-quadruplex G4 layer geometry parameters. 1-3: top layer, middle and G4 bottom, respectively.

Layers	Parameter	Crystal	Apo form	Telomestatin	TMPyP4 ¹	BSU6037 ¹	BRACO19
3:2	Rise	3.43	3.46±0.08	3.46±0.07	3.49±0.07	3.47±0.07	3.48±0.08
3:2	H-Rise	1.07	2.12±0.36	1.82±0.34	3.11±0.32	1.98±0.55	3.01±0.20
3:2	H-Twist	9.2	16.9±3.12	14.9±3.0	23.2±3.7	15.2±4.5	22.3±2.4
2:1	Rise	3.41	3.42±0.08	3.38±0.08	3.44±0.08	3.40±0.07	3.43±0.08
2:1	H-Rise	1.19	2.06±0.30	1.76±0.29	2.99±0.33	1.87±0.50	2.96±0.18
2:1	H-Twist	12.3	18.3±3.0	16.7±2.5	24.6±3.5	18.6±4.1	25.8±3.4

¹ Mean values reported for this system were calculated with consideration to the portion of the simulation where the K⁺ cation was bound inside of the structure.

Figure S1. Oxygen-Potassium Distance Parameters in the 3-layer G-quadruplex: (A) Top view of the three G4 layers. Oxygen is represented by a like colored ball, K⁺ cations are represented by a yellow ball; (B) Side view of the three G4 layers; (C) Distance (Å) of the oxygen from each residue to the nearest K⁺ cations; (D) Distance (Å) of each oxygen relative to the nearest side.

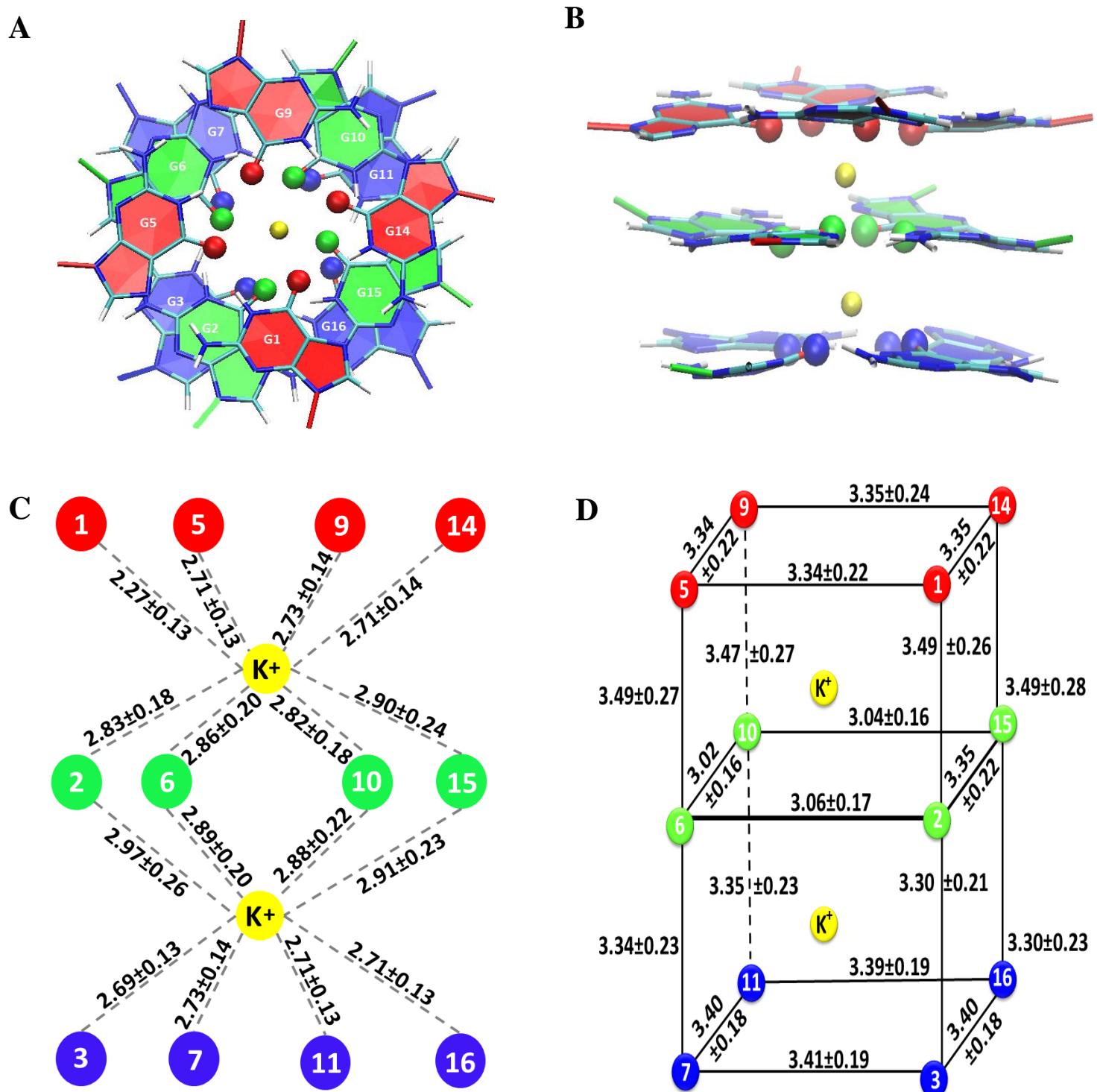


Figure S2. Initial structures of the four ligand free simulation systems. 5' and 3' are indicated by a red and blue ball, respectively. K⁺ ions are indicated by a yellow ball.

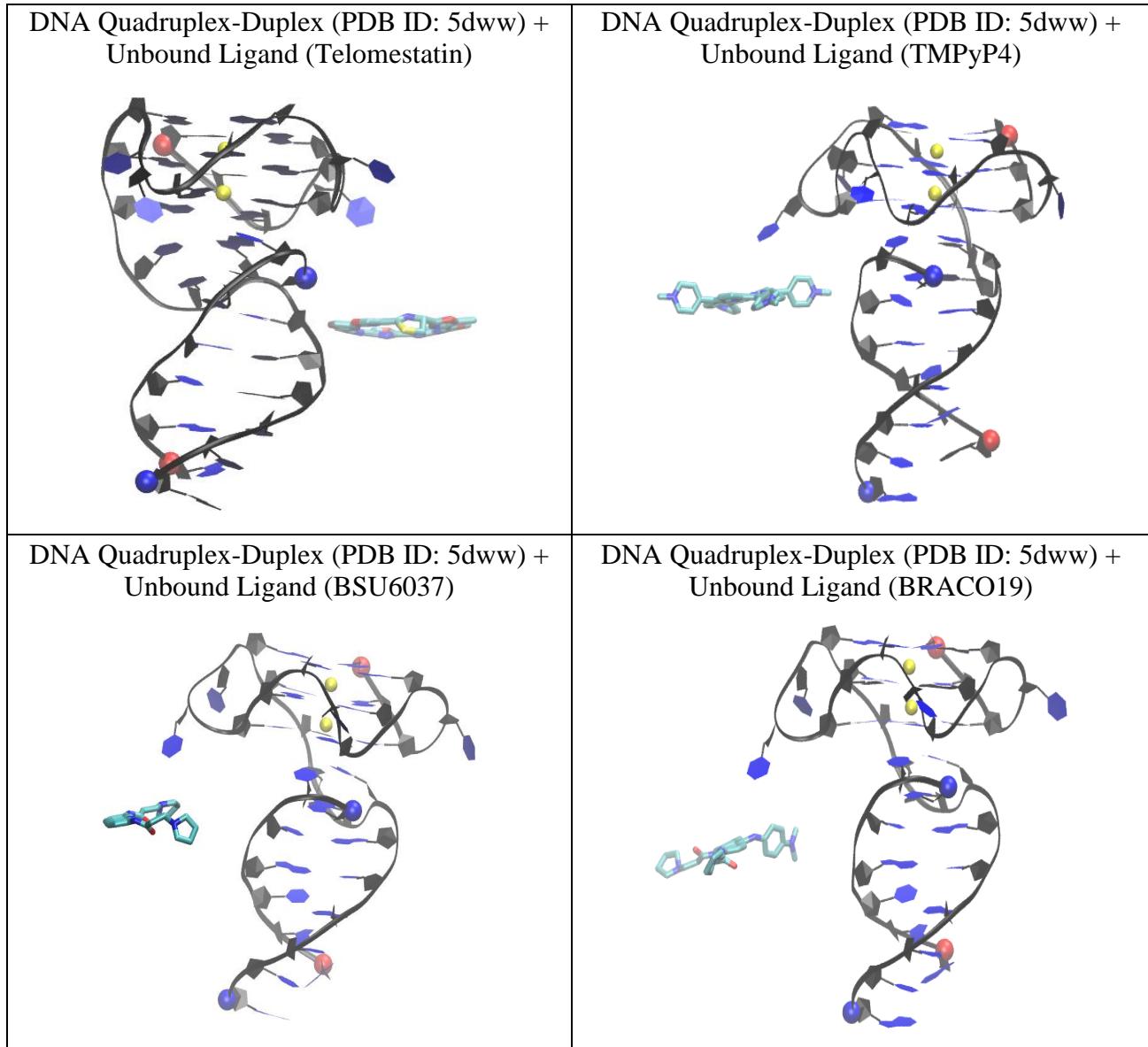


Figure S3. Average RMSD of all runs for the DNA only (1), Telomestatin only (2), TMPyP4 only (3), BSU6037 (4), and BRACO19 only (5) simulations.

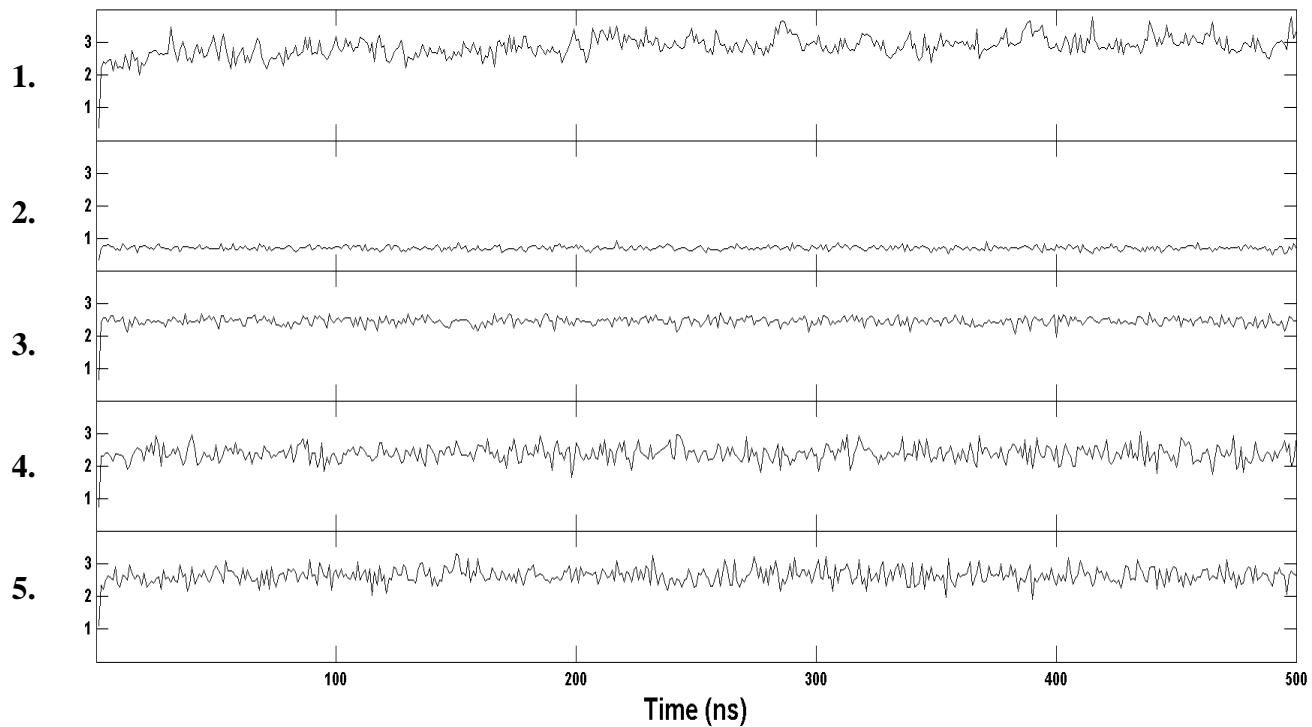


Figure S4. Average RMSD of all runs for the 5DWW/Telomestatin (1), 5DWW/TMPyP4 (2), 5DWW/BSU6037 (3), and 5DWW/BRACO19 (4) complex systems.

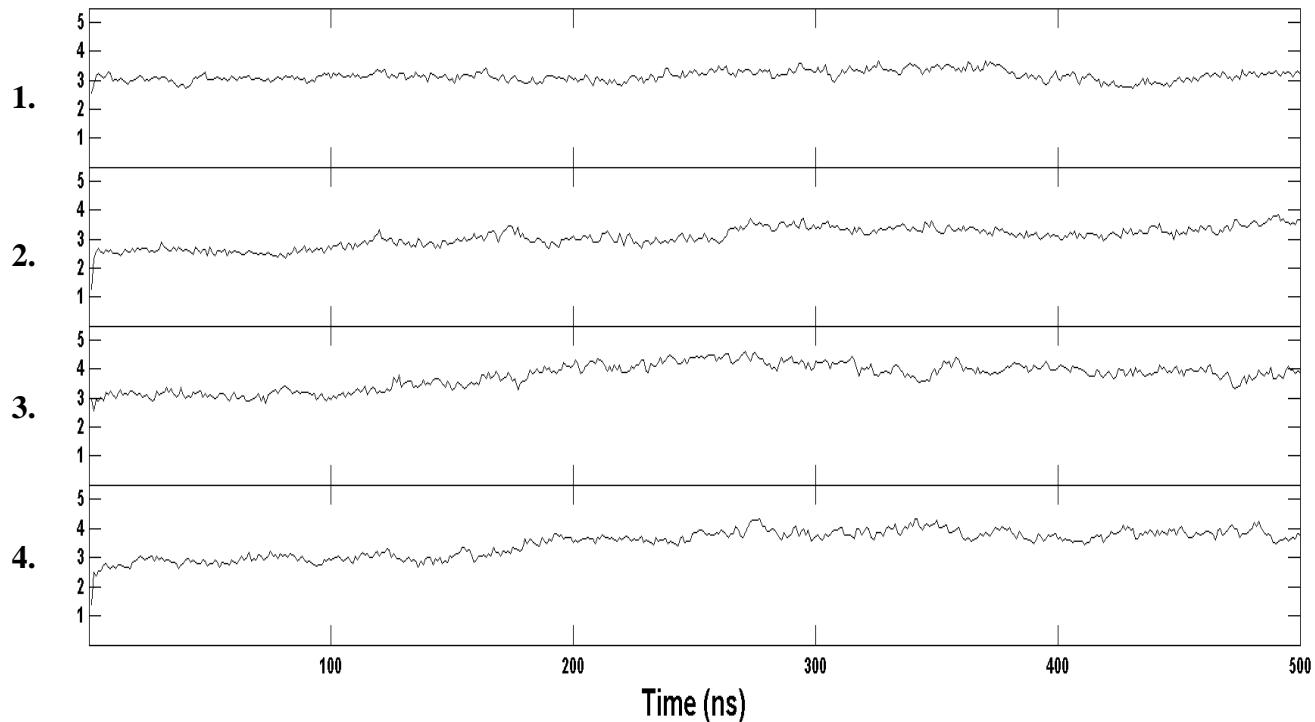


Figure S5. Average contact number of all runs between 5DWW and Telomestatin (1), TMPyP4 (2), BSU6037 (3), and BRACO19 (4).

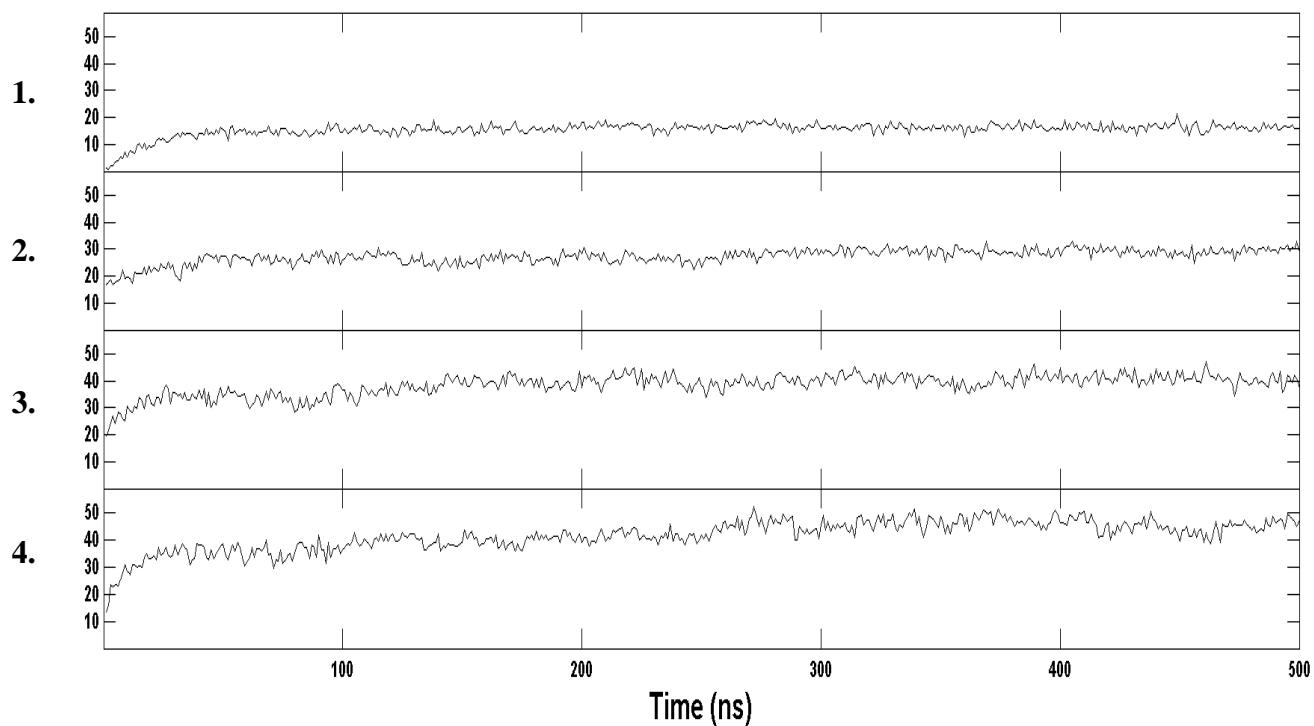


Figure S6. Last snapshots of 3 DNA only (PDB 5DWW) simulations. 5' and 3' are indicated by a red and blue ball, respectively. K⁺ ions are indicated by a yellow ball.

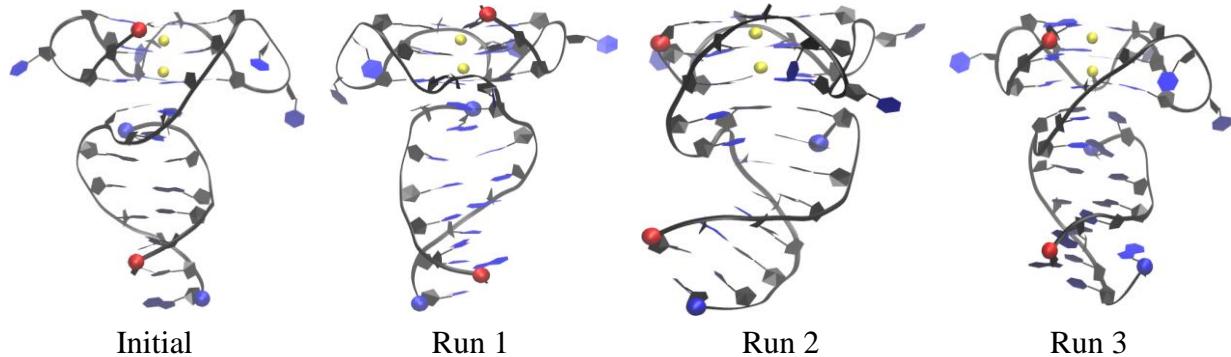
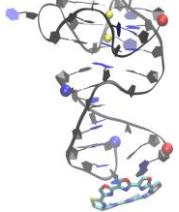
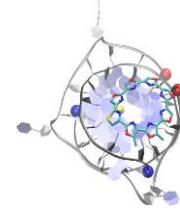
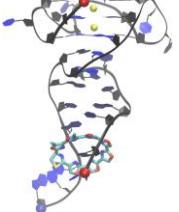
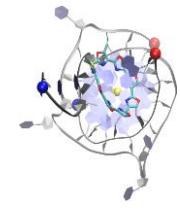
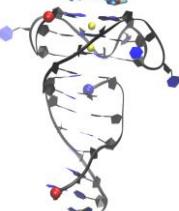
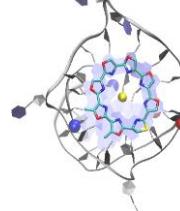
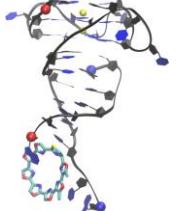
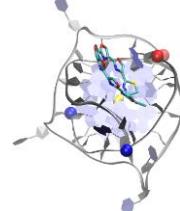
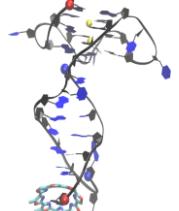
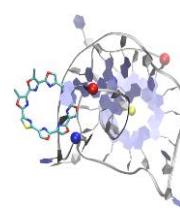
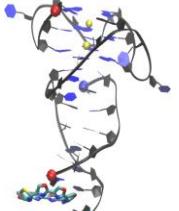
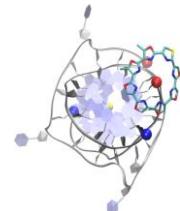
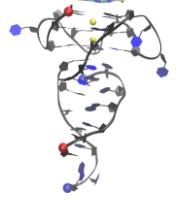
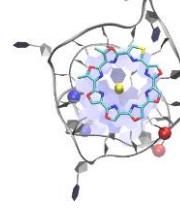
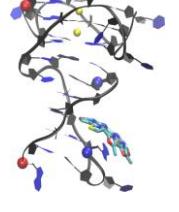
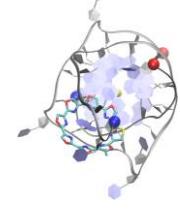
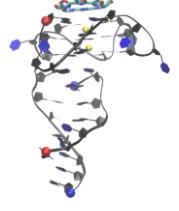
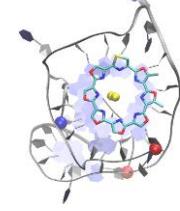
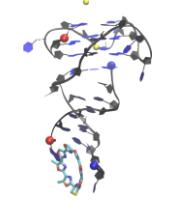
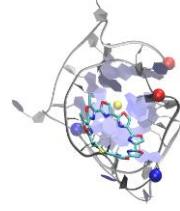


Figure S7. Final binding mode statistics of the 20 simulation runs. Reported here is the number of final binding modes of each ligand to the interface, quadruplex and duplex regions as well as the number of times a K⁺ ion moves out of the ion pore.

System	Interface	Quadruplex	Duplex	K ⁺ Ion move out
Telomestatin	0	7	13	3
TMPyP4	2	13	5	4
BSU6037	3	7	10	5
BRACO19	3	10	7	3

Figure S8. Last snapshots of 20 DNA-Telomestatin simulations. 5' and 3' are indicated by a red and blue ball, respectively. K⁺ ions are indicated by a yellow ball.

Side View	Top/Bottom View	Description (ns)	Side View	Top/Bottom View	Description (ns)
Run 01 (bottom view shown)			Run 06 (bottom view shown)		
		Duplex Stacked 6ns: quad SB, random search, 55ns: duplex stacked			Duplex Intercalated
Run 02 (top view shown)			Run 07 (bottom view shown)		
		Quadruplex Stacked 27ns: quad loop, 43ns: different quad loop, 68ns: quad stacked			Duplex Intercalated
Run 03 (bottom view shown)			Run 08 (bottom view shown)		
		Duplex Intercalated 0ns: random searching, 25ns: quad SB, 131ns: duplex intercalated, 289ns: duplex SB, 299ns: duplex intercalated			Duplex Intercalated 7ns: quad GB, 86ns: duplex binding, 136ns: duplex intercalated
Run 04 (top view shown)			Run 09 (bottom view shown)		
		Quadruplex Stacked 0ns: random searching, 107ns: quad SB, 165ns: quad stacked			Duplex Group Binding 0ns: random searching, 28ns: duplex GB
Run 05 (top view shown)			Run 10 (bottom view shown)		
		Quadruplex Stacked 0ns: random searching, 48ns: quad group binding, 199ns: quad SB, 265ns: quad stacked			Duplex Intercalated 6ns: duplex binding, 46ns: duplex intercalated

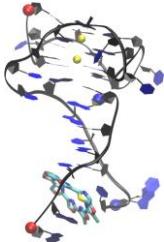
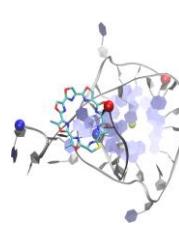
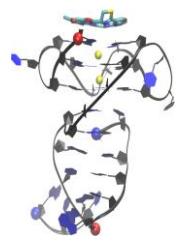
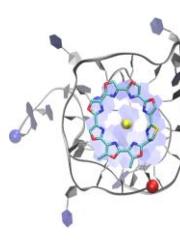
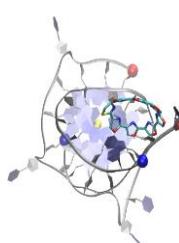
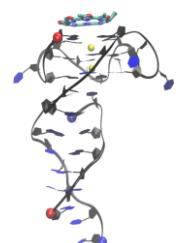
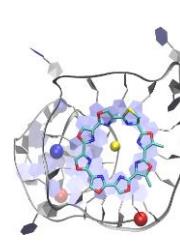
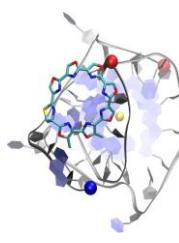
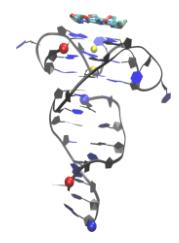
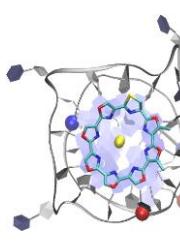
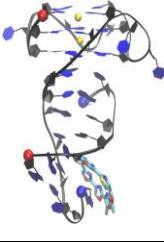
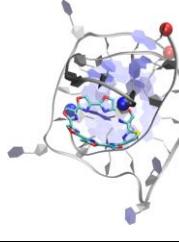
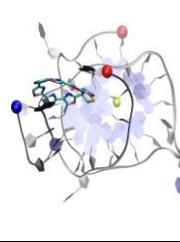
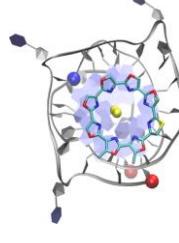
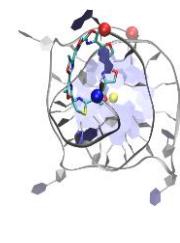
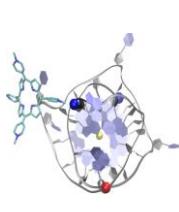
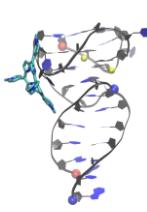
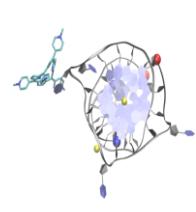
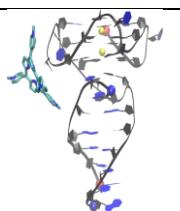
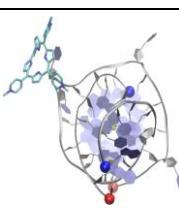
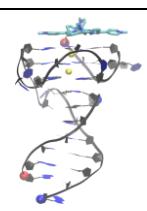
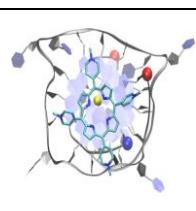
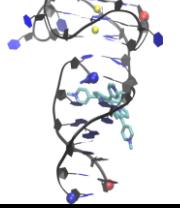
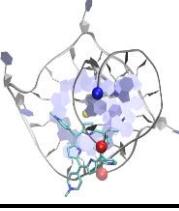
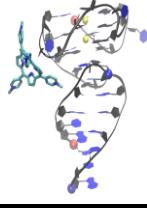
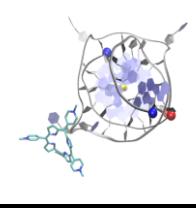
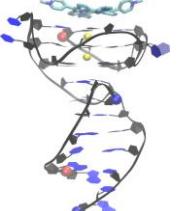
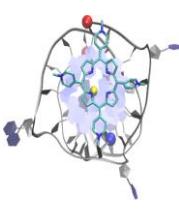
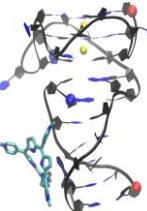
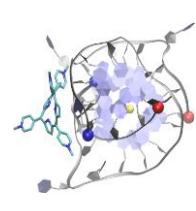
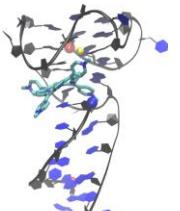
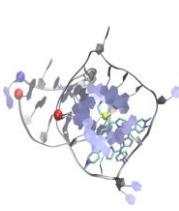
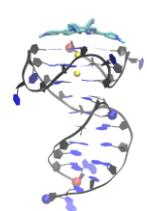
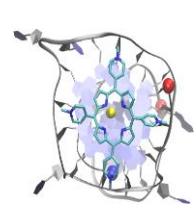
Side View	Top/Bottom View	Description (ns)	Side View	Top/Bottom View	Description (ns)
Run 11 (bottom view shown)			Run 16 (top view shown)		
		Duplex Intercalated 14ns: duplex stacked, 27ns: duplex intercalated, 84ns: duplex stacked, 395ns: duplex intercalated			Quadruplex Stacked 0ns: random searching, 25ns: quad stacked
Run 12 (bottom view shown)			Run 17 (top view shown)		
		Duplex Intercalated 3ns: quad SB, 50ns: duplex SB, random searching, 247ns: duplex intercalated			Quadruplex Stacked 6ns: duplex SB, 38ns: quad stacked
Run 13 (bottom view shown)			Run 18 (top view shown)		
		Duplex Intercalated			Quadruplex Stacked 0ns: random searching, 69ns: quad stacked
Run 14 (bottom view shown)			Run 19 (bottom view shown)		
		Duplex Intercalated			Duplex Intercalated 0ns: random searching, 29ns: duplex intercalated
Run 15 (top view shown)			Run 20 (bottom view shown)		
		Quadruplex Stacked			Duplex Intercalated 0ns: random searching, 415ns: duplex intercalated

Figure S9. Last snapshots of 20 DNA-TMPyP4 simulations. 5' and 3' are indicated by a red and blue ball, respectively. K⁺ ions are indicated by a yellow ball.

Side View	Top/Bottom View	Description (ns)	Side View	Top/Bottom View	Description (ns)
Run 01 (bottom view shown)			Run 06 (top view shown)		
		Quadruplex Side Binding			Quadruplex Side Binding 0ns: random searching, 6ns: interface interaction, 129ns: quad SB
Run 02 (bottom view shown)			Run 07 (top view shown)		
		Quadruplex Side Binding			Quadruplex Stacked 11ns: duplex intercalated, 64ns: quad stacked
Run 03 (bottom view shown)			Run 08 (bottom view shown)		
		Interface Interaction			Quadruplex Side Binding
Run 04 (top view shown)			Run 09 (bottom view shown)		
		Quadruplex Stacked 11ns: quad loop, 268ns: different quad loop, 286ns: quad stacked			Duplex Side Binding 14ns: interface interaction, 121ns: quad SB, 489ns: duplex SB
Run 05 (top view shown)			Run 10 (top view shown)		
		Interface Interaction 17ns: quad SB, 56ns: interface interaction			Quadruplex Stacked 8ns: interface interaction, 44ns: quad stacked

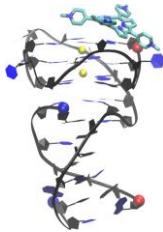
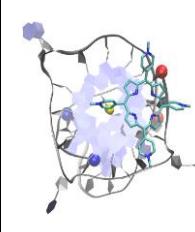
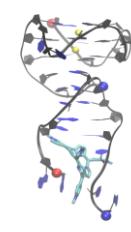
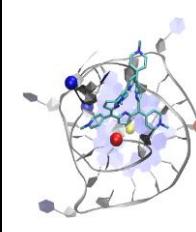
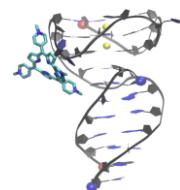
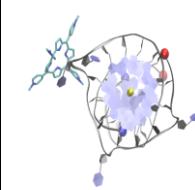
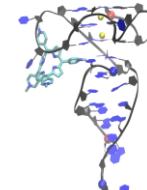
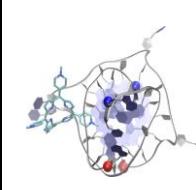
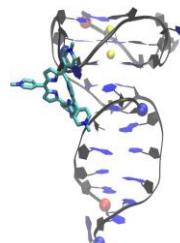
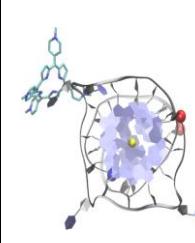
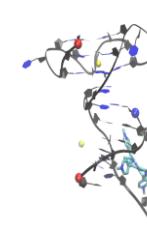
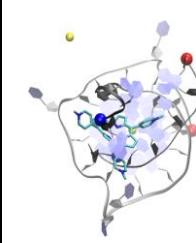
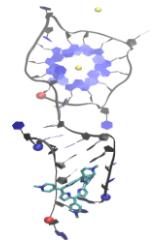
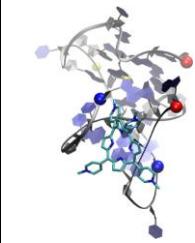
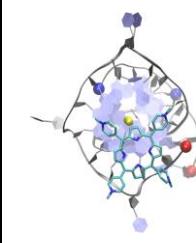
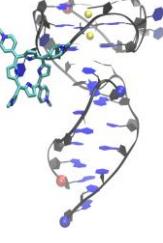
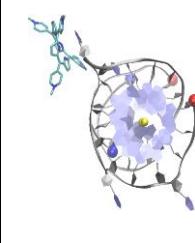
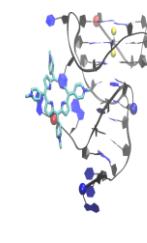
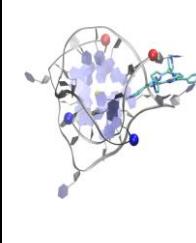
Side View	Top/Bottom View	Description (ns)	Side View	Top/Bottom View	Description (ns)
Run 11 (top view shown)			Run 16 (bottom view shown)		
		Quadruplex Stacked 6ns: quad SB, 14ns: quad stacked			Duplex Intercalated 0ns: random searching, 38ns: duplex intercalated
Run 12 (top view shown)			Run 17 (bottom view shown)		
		Quadruplex Side Binding			Quadruplex Side Binding 0ns: random searching, 41ns: quad SB
Run 13 (top view shown)			Run 18 (bottom view shown)		
		Quadruplex Side Binding			Duplex Intercalated
Run 14 (bottom view shown)			Run 19 (top view shown)		
		Duplex Intercalated 0ns: random searching, 44ns: duplex intercalated			Quadruplex Stacked 0ns: random searching, 18ns: quad stacked
Run 15 (top view shown)			Run 20 (bottom view shown)		
		Quadruplex Side Binding			Quadruplex+Duplex Binding 0ns: random searching, 198ns: binding to quadruplex residue and side of duplex

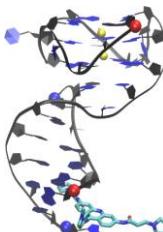
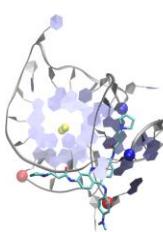
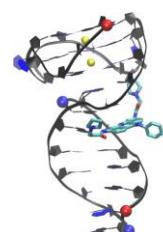
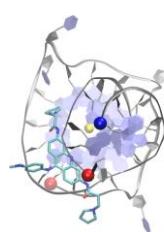
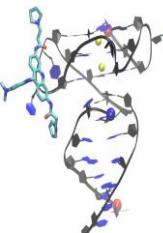
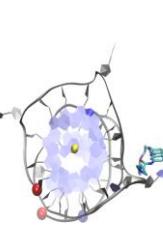
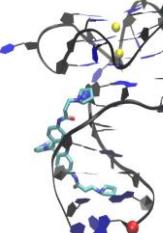
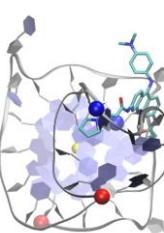
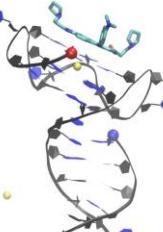
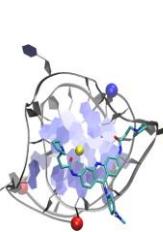
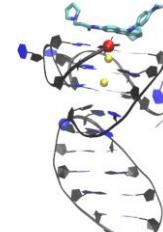
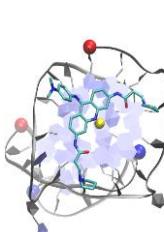
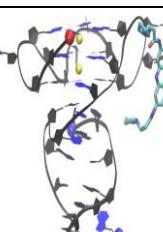
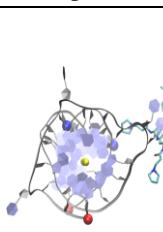
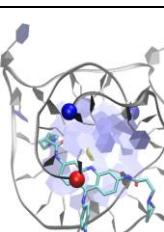
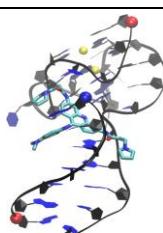
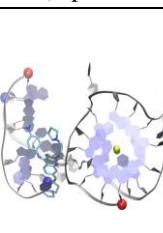
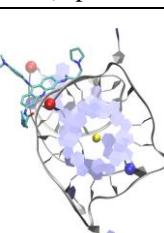
Figure S10. Last snapshots of 20 DNA-BSU6037 simulations. 5' and 3' are indicated by a red and blue ball, respectively. K⁺ ions are indicated by a yellow ball.

Side View	Top/Bottom View	Description (ns)	Side View	Top/Bottom View	Description (ns)
Run 01 (top view shown)			Run 06 (top view shown)		
		Quadruplex Group Binding 13ns: quad SB, 124ns: interface SB, 321ns: quad SB, 395ns: quad GB			Quadruplex Side Binding 0ns: random searching, 435ns: quad stacking, 481ns: quad SB
Run 02 (top view shown)			Run 07 (top view shown)		
		Quadruplex Stacking 0ns: random searching, 114ns: quad stacking			Interface Intercalating 0ns: random searching, 51ns: quad GB, 174ns: interface SB, 323ns: interface intercalating
Run 03 (bottom view shown)			Run 08 (bottom view shown)		
		Duplex Group Binding 0ns: random searching, 83ns: duplex GB, 156ns: duplex groove (group binding)			Duplex Side Binding 13ns: quad SB, 440ns: duplex SB
Run 04 (bottom view shown)			Run 09 (top view shown)		
		Duplex Intercalating 9ns: interface SB, 4ns: duplex intercalating and remains			Quadruplex Group Binding 0ns: random searching, 327ns: quad GB
Run 05 (bottom view shown)			Run 10 (bottom view shown)		
		Duplex Intercalating 0ns: random searching, 23ns: quad SB, 110ns: duplex intercalating			Duplex Intercalating

Side View	Top/Bottom View	Description (ns)	Side View	Top/Bottom View	Description (ns)
Run 11 (bottom view shown)			Run 16 (bottom view shown)		
		Duplex Group Binding			Duplex Intercalating 0ns: random searching, 317ns: duplex intercalating
Run 12 (bottom view shown)			Run 17 (top view shown)		
		Duplex Intercalating 0ns: random searching, 123ns: duplex intercalating			Quadruplex Stacking 0ns: random searching, 365ns: quad GB, 374ns: quad stacking
Run 13 (top view shown)			Run 18 (top view shown)		
		Quadruplex Group Binding			Quadruplex Group Binding 0ns: random searching, 3ns: quad SB, 37ns: duplex SB, 449ns: quad GB
Run 14 (bottom view shown)			Run 19 (bottom view shown)		
		Interface Side Binding 0ns: random searching, 4ns: quad SB, 180ns: changes configuration shape, 470ns: interface SB			Interface Stacking 0ns: random searching, 250ns: interface stacking
Run 15 (bottom view shown)			Run 20 (bottom view shown)		
		Duplex Stacking 0ns: random searching, 167ns: duplex SB, 177ns: duplex stacking			Duplex Intercalating 0ns: random searching, 115ns: duplex intercalating

Figure S11. Last snapshots of 20 DNA-BRACO19 simulations. 5' and 3' are indicated by a red and blue ball, respectively. K⁺ ions are indicated by a yellow ball.

Side View	Top/Bottom View	Description (ns)	Side View	Top/Bottom View	Description (ns)
Run 01 (bottom view shown)			Run 06 (bottom view shown)		
		Duplex Group Binding 0ns: random searching, 263ns: duplex GB			Interface Interaction 15ns: quad SB, 101ns: quad GB
Run 02 (top view shown)			Run 07 (bottom view shown)		
		Quadruplex Stacking 0ns: random searching, 63ns: quad SB, 407ns: quad stacking			Quadruplex side binding 12ns: quad GB, 153ns: Quadruplex side binding
Run 03 (top view shown)			Run 08 (bottom view shown)		
		Quadruplex Group Binding 0ns: random searching, 7ns: quad GB			Interface Side Binding 0ns: random searching, 7ns: duplex GB, 18ns: interface SB
Run 04 (bottom view shown)			Run 09 (bottom view shown)		
		Duplex Stacking 0ns: random searching, 430ns: duplex stacking			Quadruplex Group Binding 0ns: random searching, 5ns: interface GB and remains
Run 05 (top view shown)			Run 10 (top view shown)		
		Quadruplex Stacking 0ns: random searching, 7ns: quad SB			Interface Interaction 0ns: random searching, 63ns: interface interaction and remains

Side View	Top/Bottom View	Description (ns)	Side View	Top/Bottom View	Description (ns)
Run 11 (bottom view shown)			Run 16 (bottom view shown)		
		Duplex Group Binding 0ns: random searching, 87ns: duplex GB and remains			Duplex Binding
Run 12 (top view shown)			Run 17 (bottom view shown)		
		Quadruplex Side Binding 17ns: interface SB, 306ns: quad SB			Duplex Group Binding 0ns: random searching, 47ns: duplex stacking, 180ns: duplex GB
Run 13 (top view shown)			Run 18 (top view shown)		
		Quadruplex Stacking 0ns: random searching, 7ns: quad stacking and remains			Quadruplex Stacking
Run 14 (top view shown)			Run 19 (bottom view shown)		
		Quadruplex Group Binding 0ns: random searching, 143ns: quad GB			Duplex Group Binding 0ns: random searching, 88ns: duplex GB and remains
Run 15 (top view shown)			Run 20 (top view shown)		
		Duplex Binding 0ns: random searching, 15ns: duplex binding+interface interaction, 180ns: duplex binding			Quadruplex binding 0ns: random searching, 98ns: Quadruplex binding

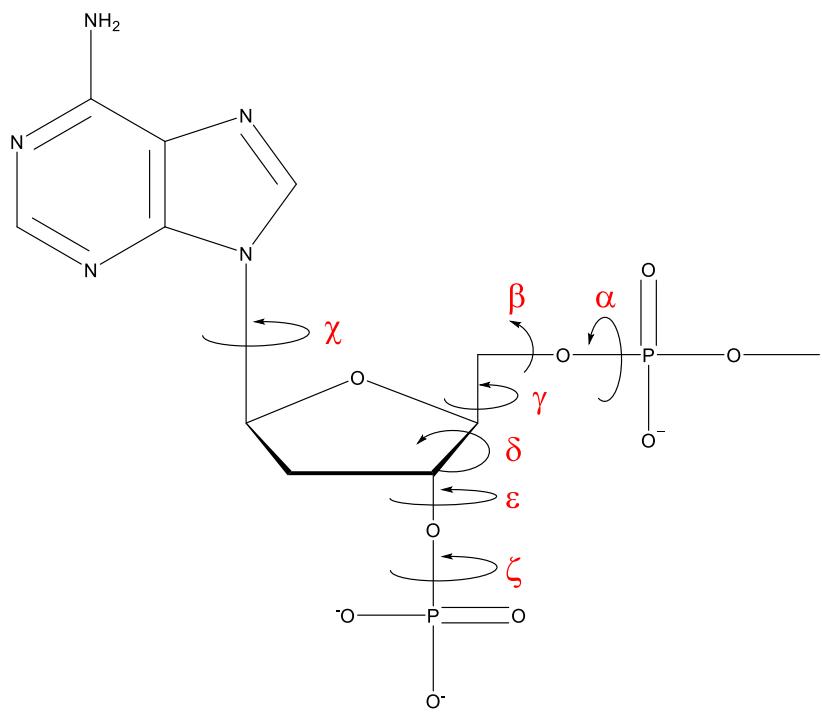
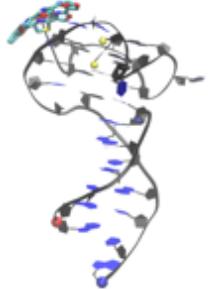
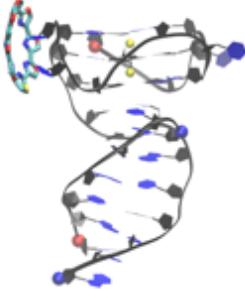


Figure S12. Backbone Torsion Angles of DNA.

Figure S13. Clustering analysis. In this table, total refers to the total number of analyzed conformations per system (20 x 500 ns). The stable complex and percentage quantify the stable complexes considered in the clustering analysis. Cluster number refers to the reported clusters that are statistically significant (within 1% of the total of stable complexes). The number of stable complexes per cluster indicates the number of conformations out of the total number of stable complexes that are classified into one structural family.

	Telomestatin	TMPyP4	BSU6037	BRACO19
Total	10,000	10,000	10,000	10,000
Stable Complexes	1964	3418	4934	6289
Percentage	19.6%	34.2%	49.3 %	62.9 %
Cluster #	Number of Stable Complexes Per Cluster			
1	662	602	1826	824
2	170	556	444	716
3	84	460	354	584
4	16	376	300	448
5	16	292	270	336
6	10	270	230	292
7	6	246	176	256
8	6	102	148	196
9	4	86	120	164
10	2	56	112	160
11	2	38	98	132
12	2	36	90	128

Figure S14. Representative structures of the most populated complex structure families (population $\geq 1\%$) from the clustering analysis of the combined binding trajectories. 5' and 3' are indicated by a red and blue ball, respectively, for Telomestatin binding to the quadruplex and duplex. K⁺ ions are indicated by a yellow ball.

Binding model	Quadruplex	
Cluster ID	C1	C2
Representative Structure (Side View)		
Population	35%	5%

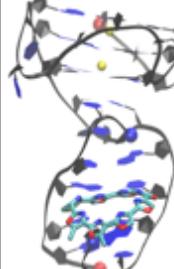
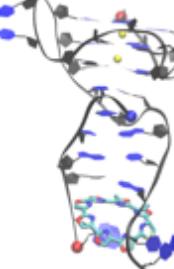
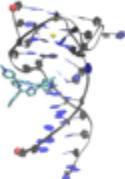
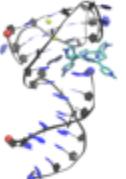
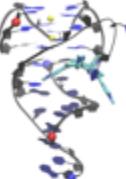
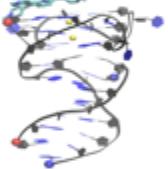
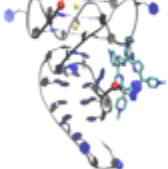
Binding model	Duplex			
Cluster ID	A1	A2	A3	A4
Representative Structure (Side View)				
Population	30%	10%	9%	2%

Figure S15. Representative structures of the most populated complex structure families (population $\geq 1\%$) from the clustering analysis of the combined binding trajectories. 5' and 3' are indicated by a red and blue ball, respectively, for **TMPyP4** interacting with the interface, quadruplex, and duplex. K⁺ ions are indicated by a yellow ball.

Binding model	Interface			
Cluster ID	A1	A2	A3	A4
Representative Structure (Side View)				
Population	13%	8%	8%	2%

Binding model	Quadruplex		Binding model	Duplex+Quadruplex
Cluster ID	B1		Cluster ID	C1
Representative Structure (Side View)			Representative Structure (Side View)	
Population	17%		Population	7%

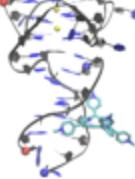
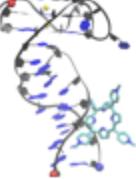
Binding model	Duplex		
Cluster ID	D1	D2	D3
Representative Structure (Side View)			
Population	16%	11%	3%

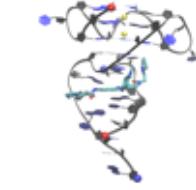
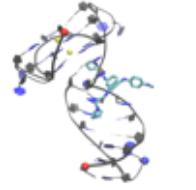
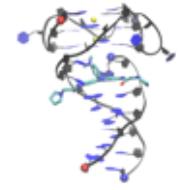
Figure S16. Representative structures of the most populated complex structure families (population $\geq 1\%$) from the clustering analysis of the combined binding trajectories. 5' and 3' are indicated by a red and blue ball, respectively, for BSU6037 binding to the interface, quadruplex, and duplex. K⁺ ions are indicated by a yellow ball.

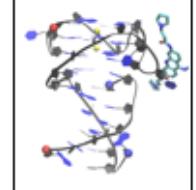
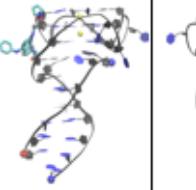
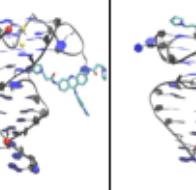
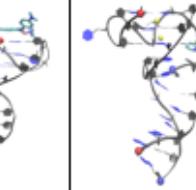
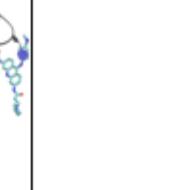
Binding model	Interface	
Cluster ID	A1	A2
Representative Structure (Side View)		
Population	3%	2%

Binding model	Quadruplex		
Cluster ID	B1	B2	B3
Representative Structure (Side View)			
Population	7%	3%	2%

Binding model	Duplex				
Cluster ID	C1	C2	C3	C4	C5
Representative Structure (Side View)					
Population	36%	9%	6%	5%	5%

Figure S17. Representative structures of the most populated complex structure families (population $\geq 1\%$) from the clustering analysis of the combined binding trajectories. 5' and 3' are indicated by a red and blue ball, respectively, for BRACO19 interacting with the interface, quadruplex, and duplex. K⁺ ions are indicated by a yellow ball.

Binding model	Interface		
Cluster ID	A1	A2	A3
Representative Structure (Side View)			
Population	17%	7%	5%

Binding model	Quadruplex				
Cluster ID	B1	B2	B3	B4	B5
Representative Structure (Side View)					
Population	11%	9%	5%	3%	3%

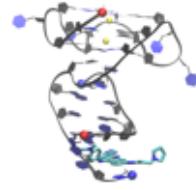
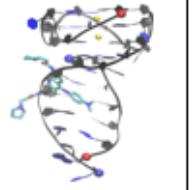
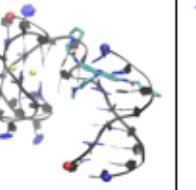
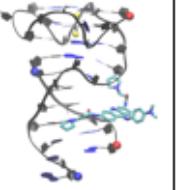
Binding model	Duplex			
Cluster ID	C1	C2	C3	C4
Representative Structure (Side View)				
Population	13%	4%	3%	2%

Figure S18. H-bond network in the 5 layers (3 G-tetrad, 2 Dyad) formed by DNA residues in the interface binding modes (Figure 4).

H-bonds	G-tetrad (1)	G-tetrad (2)	G-tetrad (3)	Dyad1	Dyad2
(A) TMPyP4	G5 G9 G1 G14	G6 G10 G2 G15	G7 G3 G11 G16	T19 T17	A18 T7
(B) BSU6037	G5 G9 G1 G14	G6 G10 G2 G15	G7 G3 G11 G16	A8 T17	A18 T7

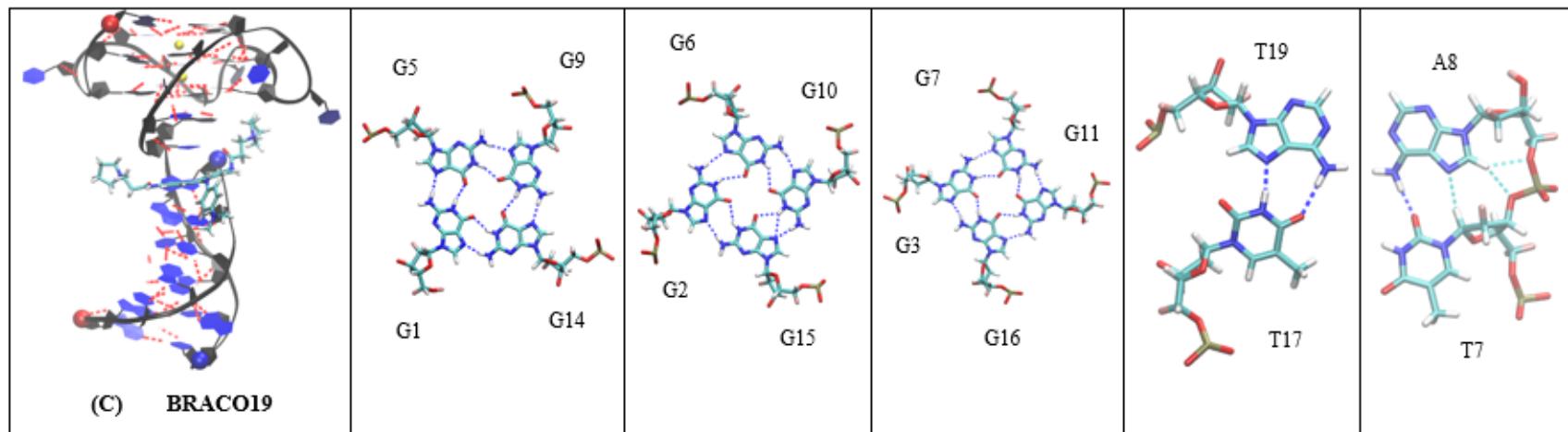


Figure S19. 2D ligand-DNA interactions in the major binding modes between ligands and human telomeric quadruplex-duplex.

	Interface	Quadruplex	Duplex
Telomestatin (A)	N/A		
TMPyP4 (B)			

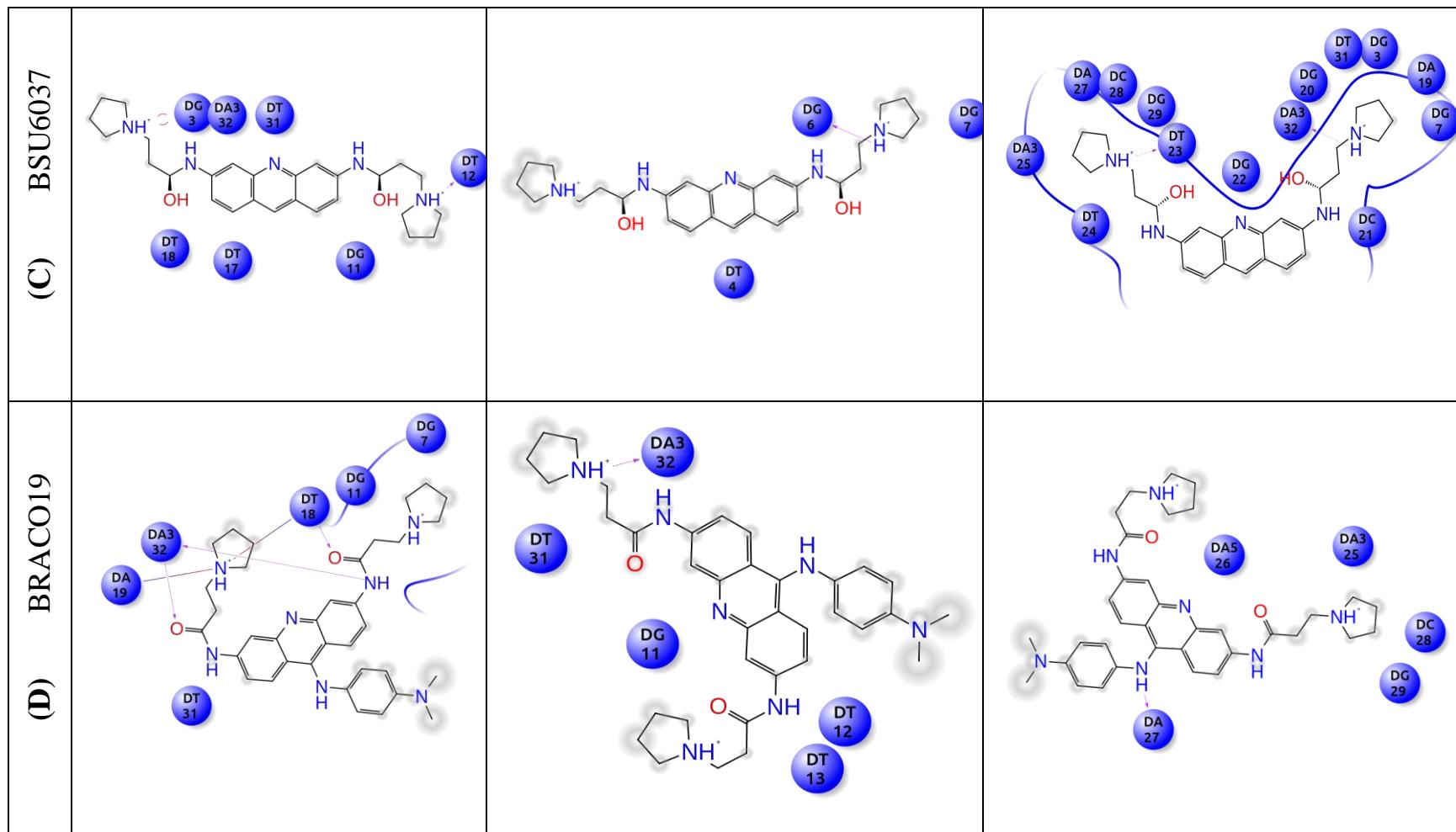


Figure S20. Telomestatin, run 9, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

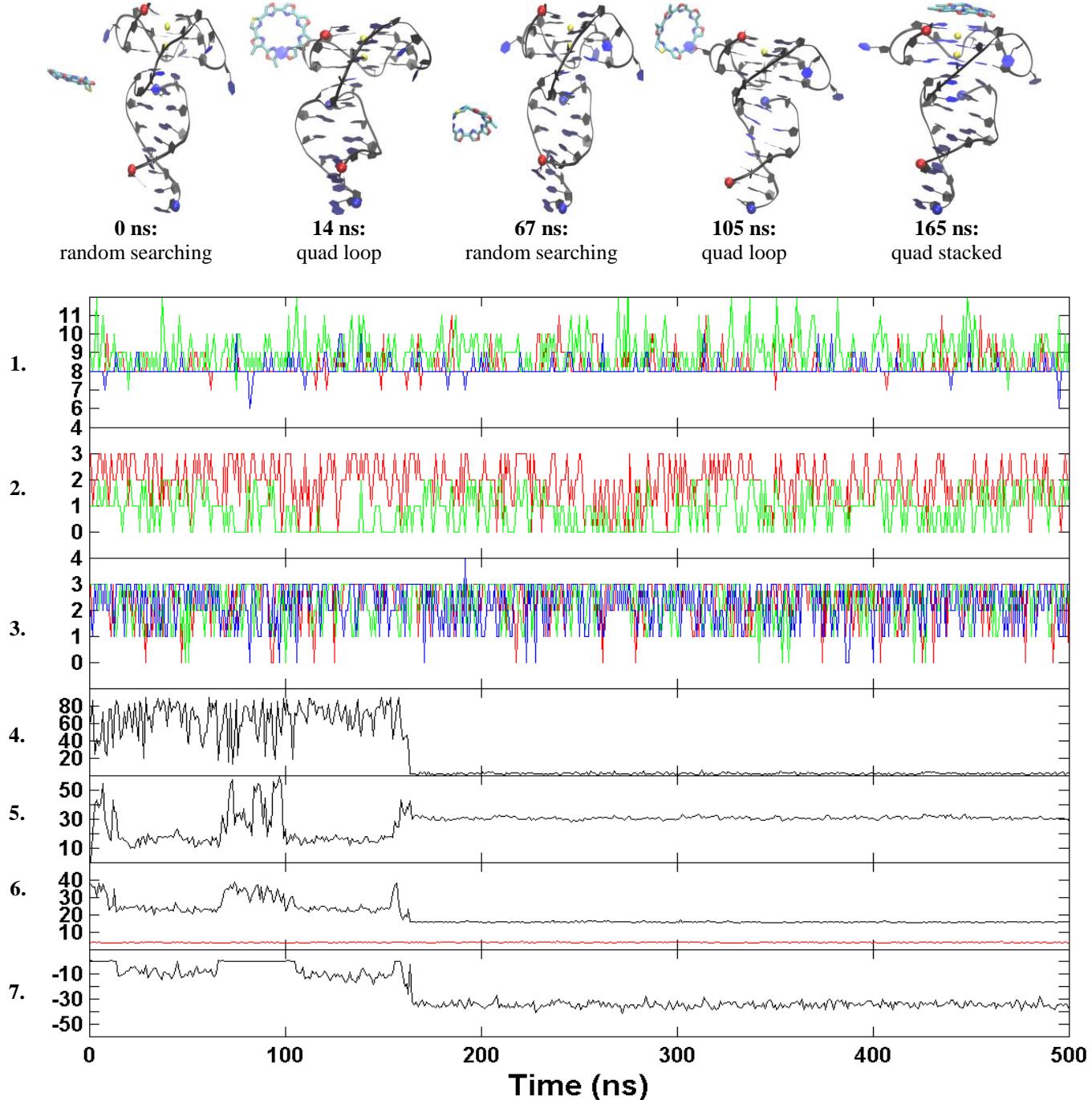


Figure S21. Telomestatin, run 1, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

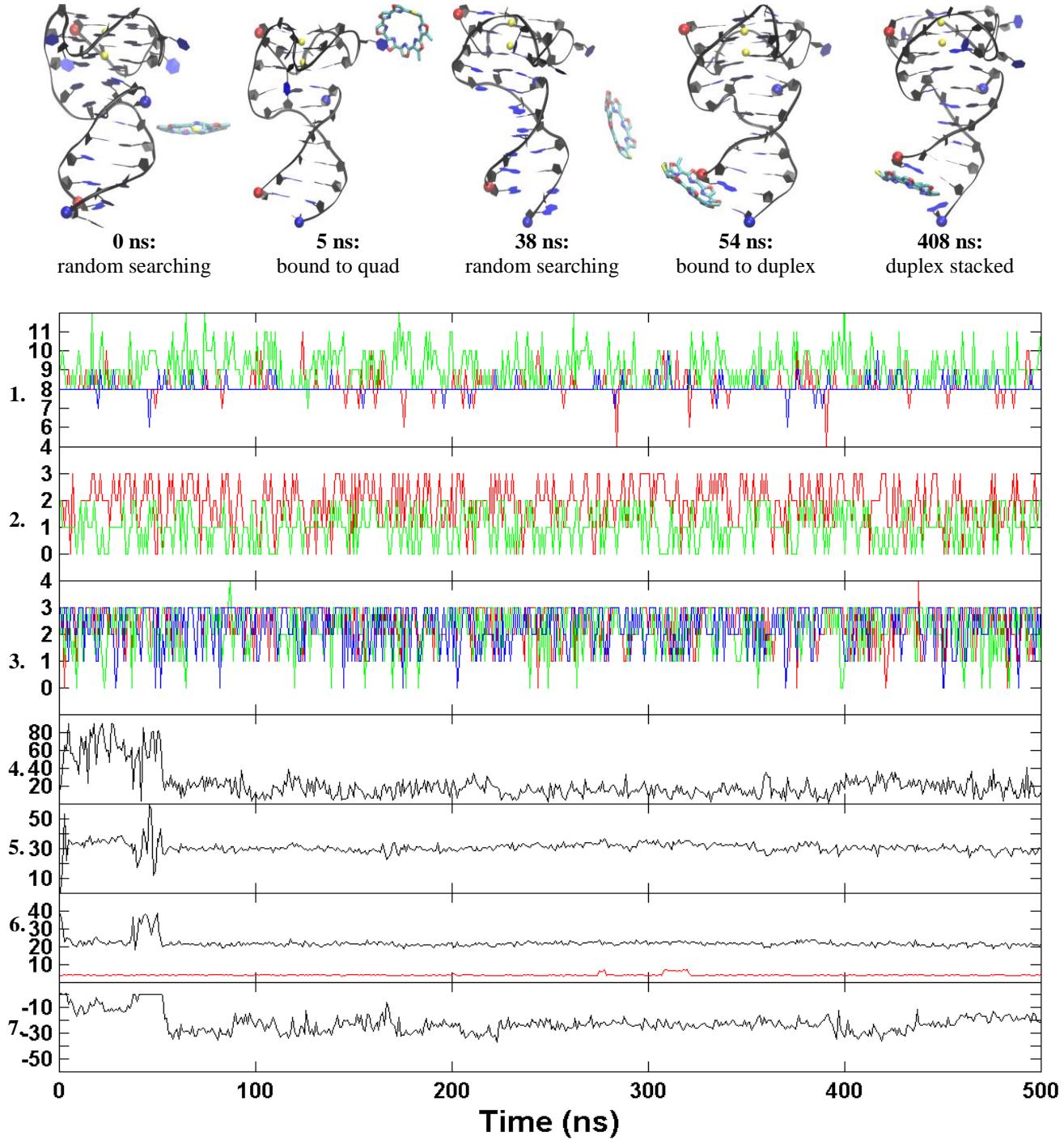


Figure S22. TMPyP4, run 3, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen-bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center(black) and K⁺ to K⁺ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K⁺ ions are indicated by yellow balls.

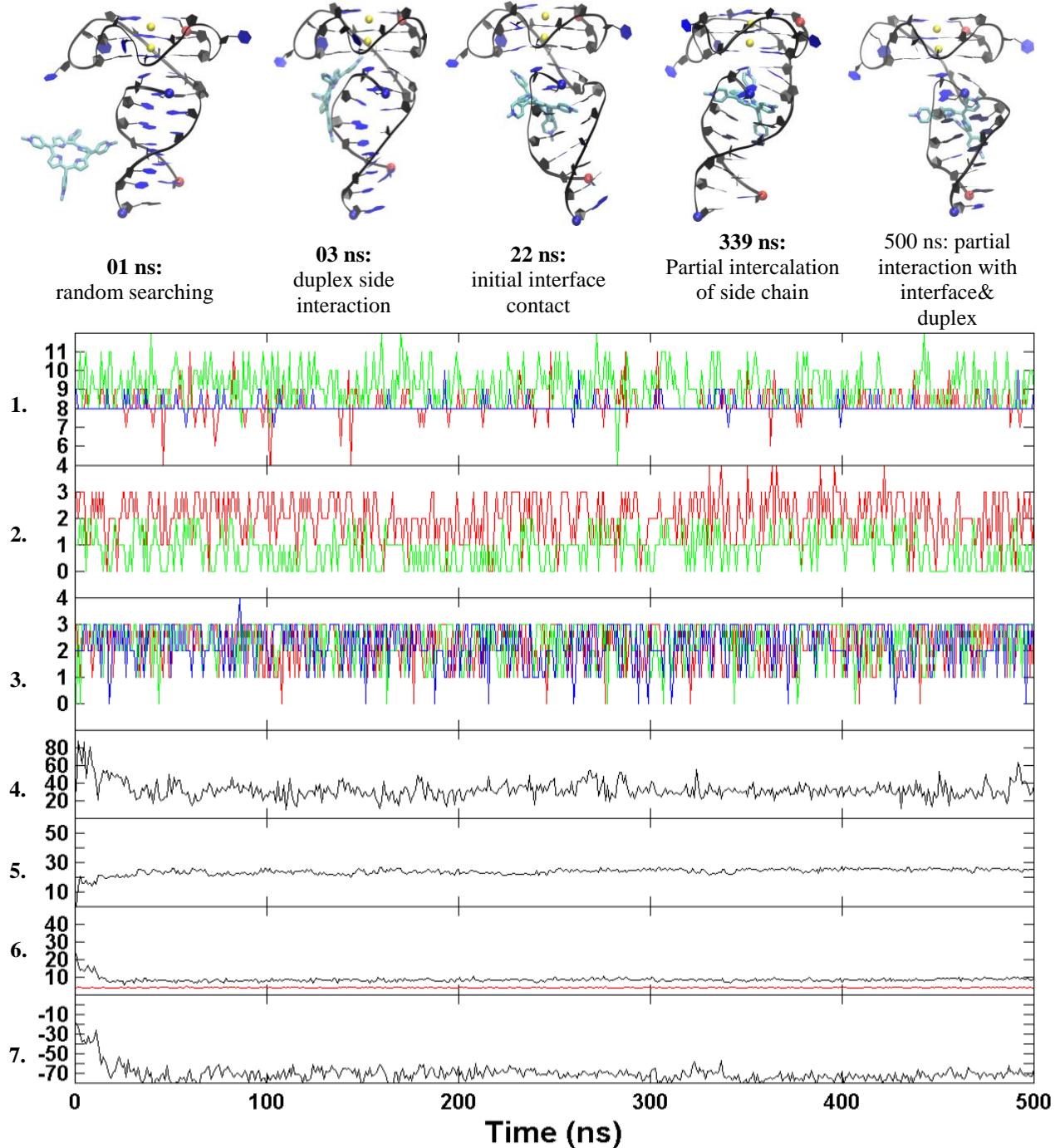


Figure S23. TMPyP4, run 19, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

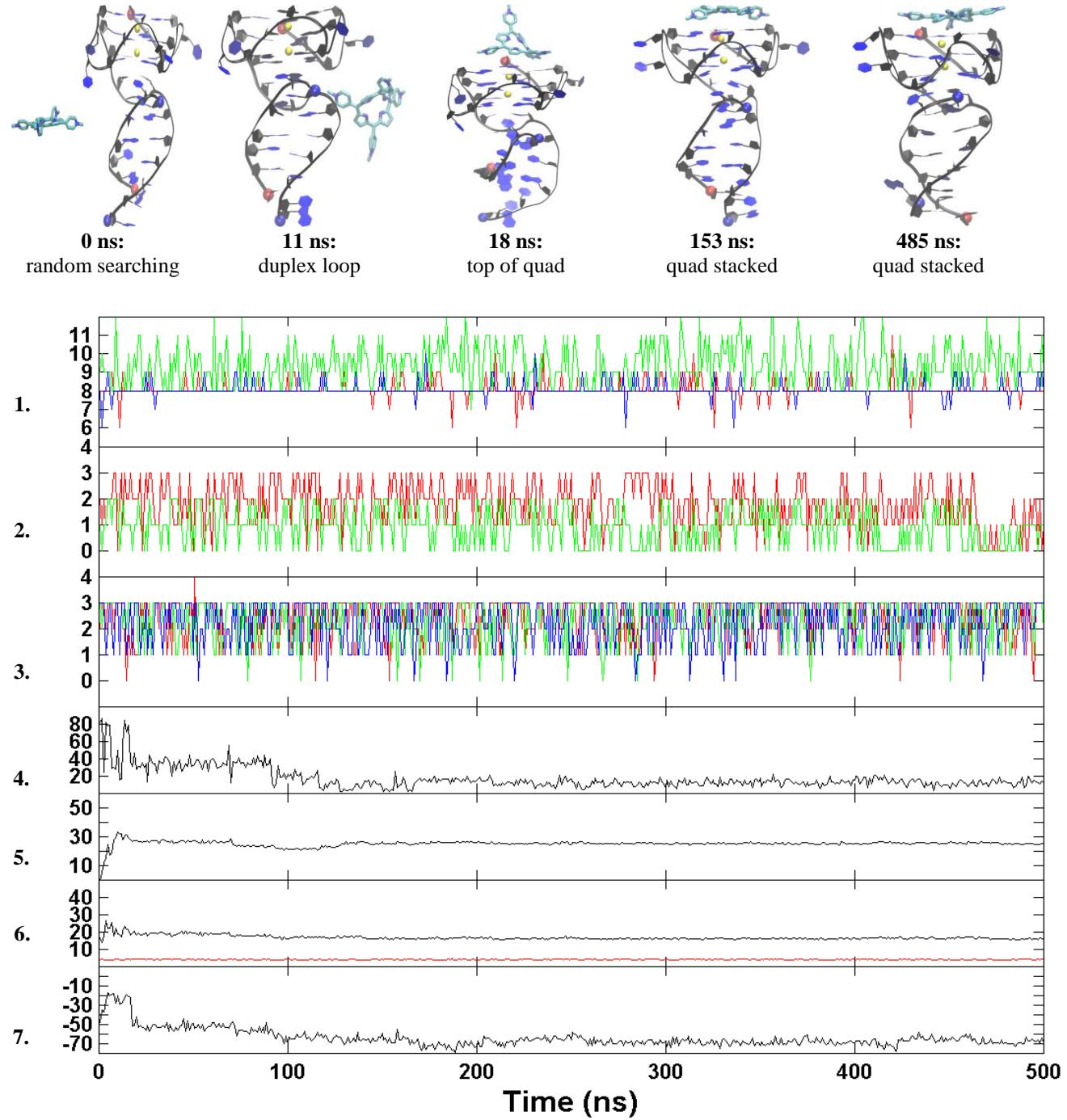


Figure S24. TMPyP4, run 18, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

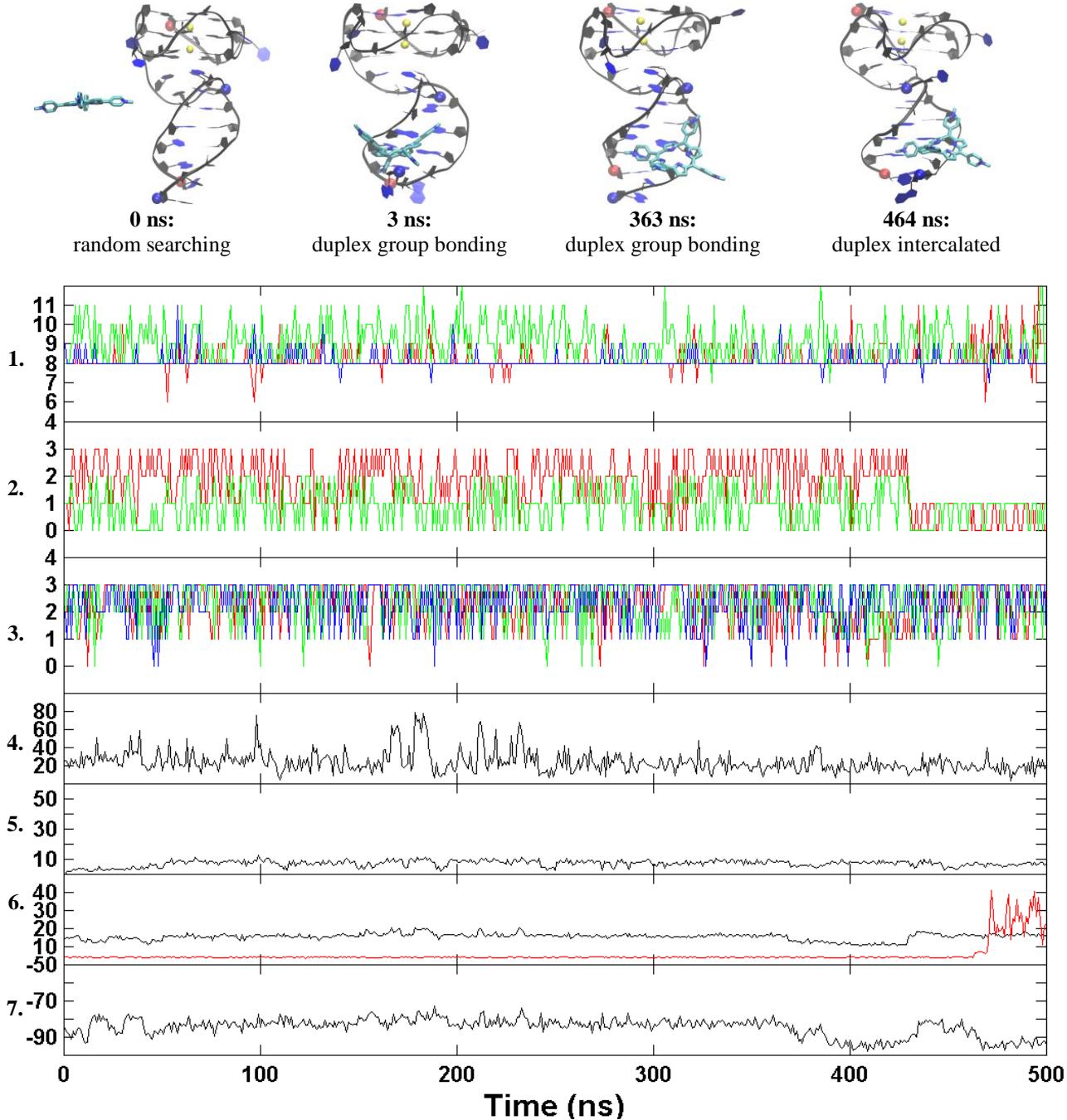


Figure S25. BSU6037, (run 7), trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K⁺ to K⁺ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K⁺ ions are indicated by yellow balls.

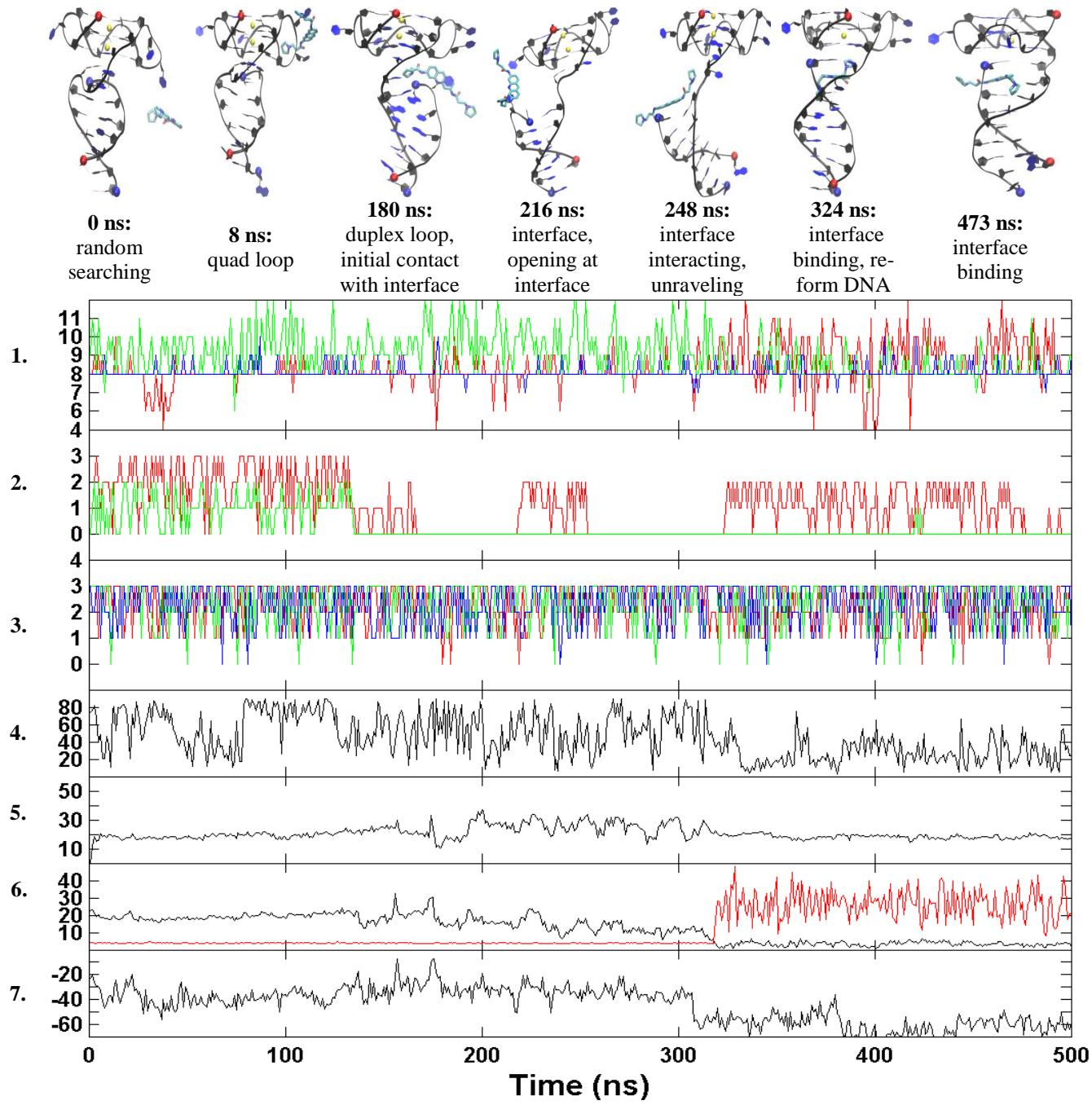


Figure S26. BSU6037, run 18, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

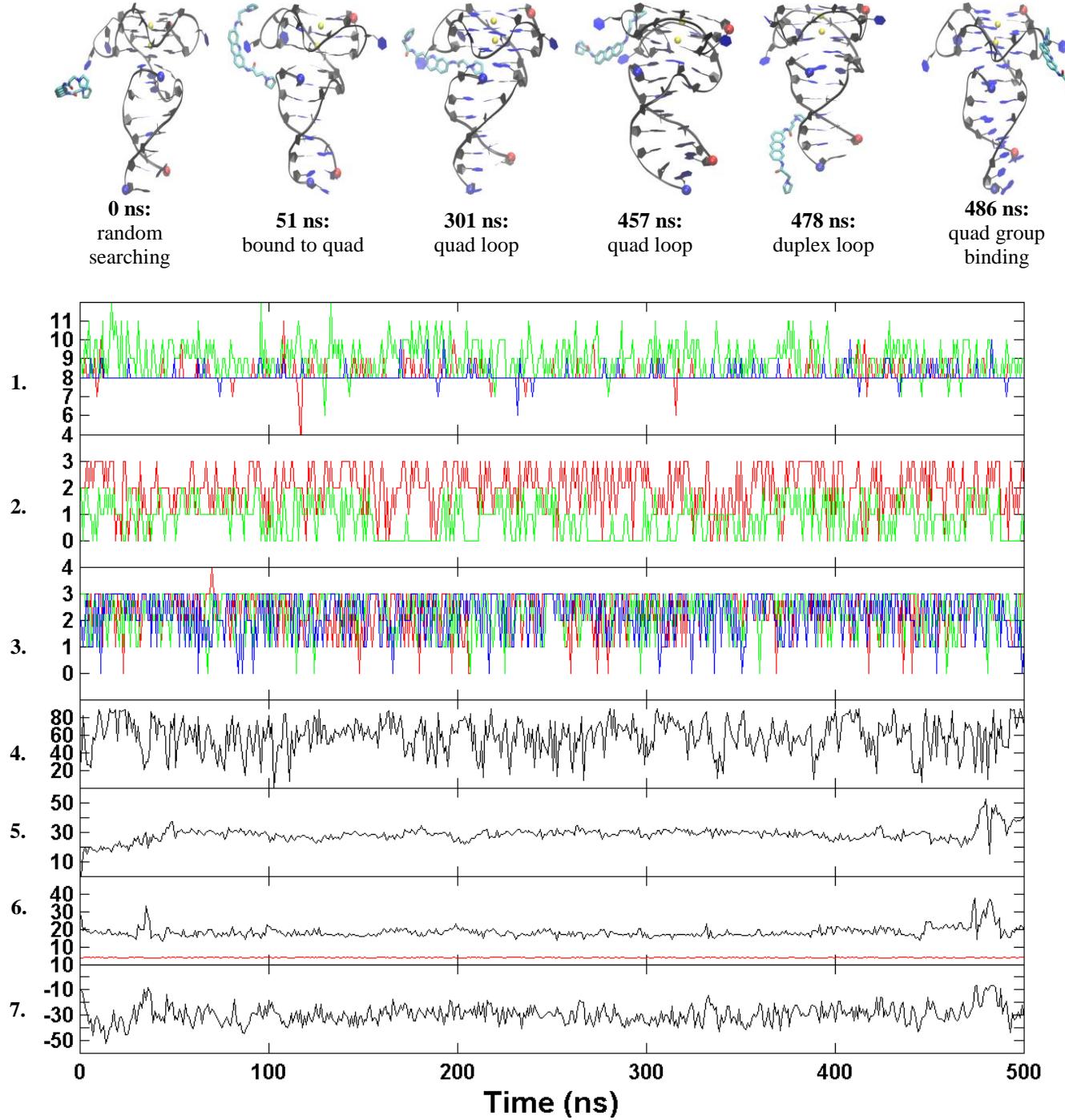


Figure S27. BSU6037, run 3, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center(distance(black) and K⁺ to K⁺ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K⁺ ions are indicated by yellow balls.

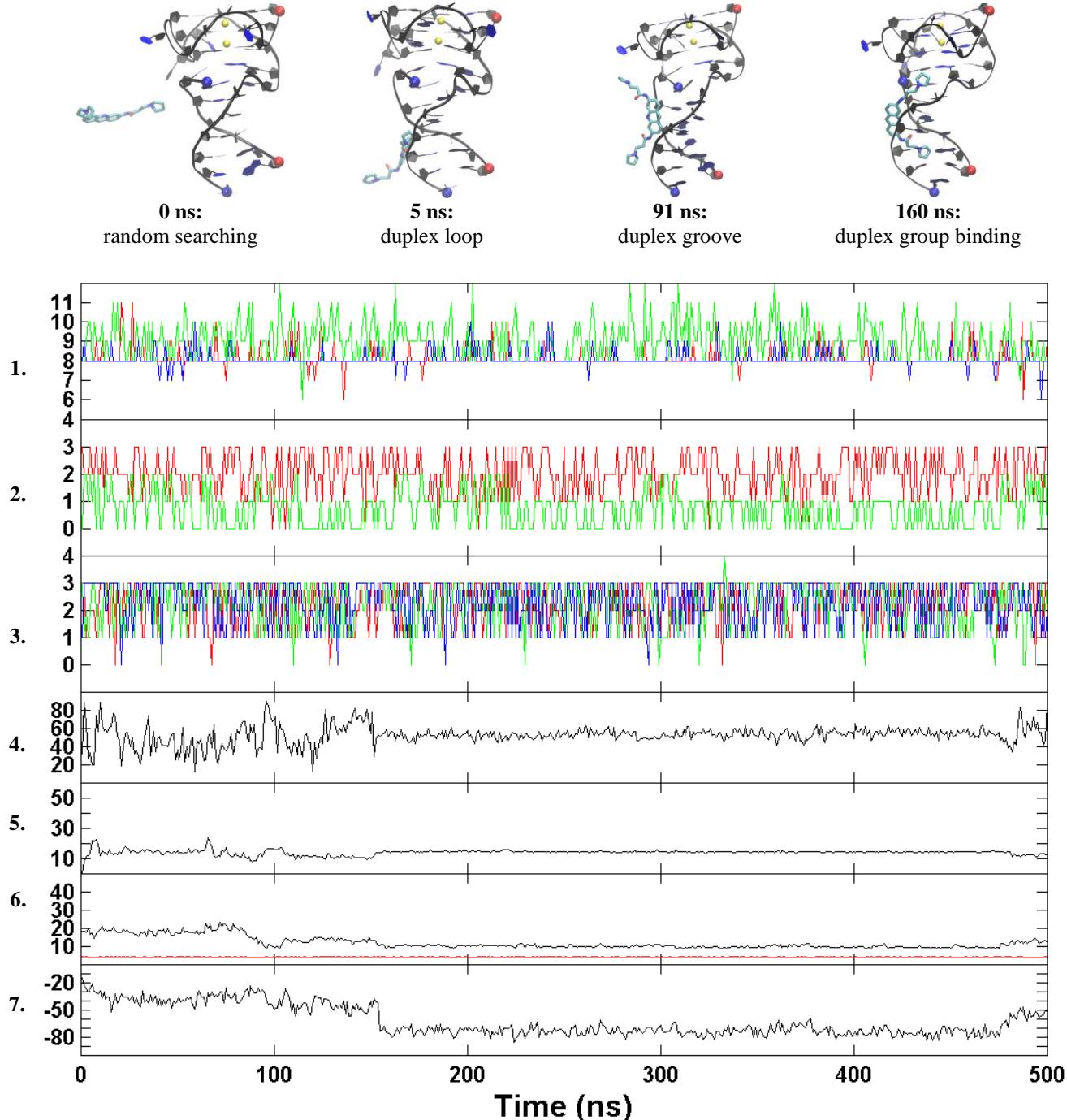


Figure S28. BRACO19, run 8, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

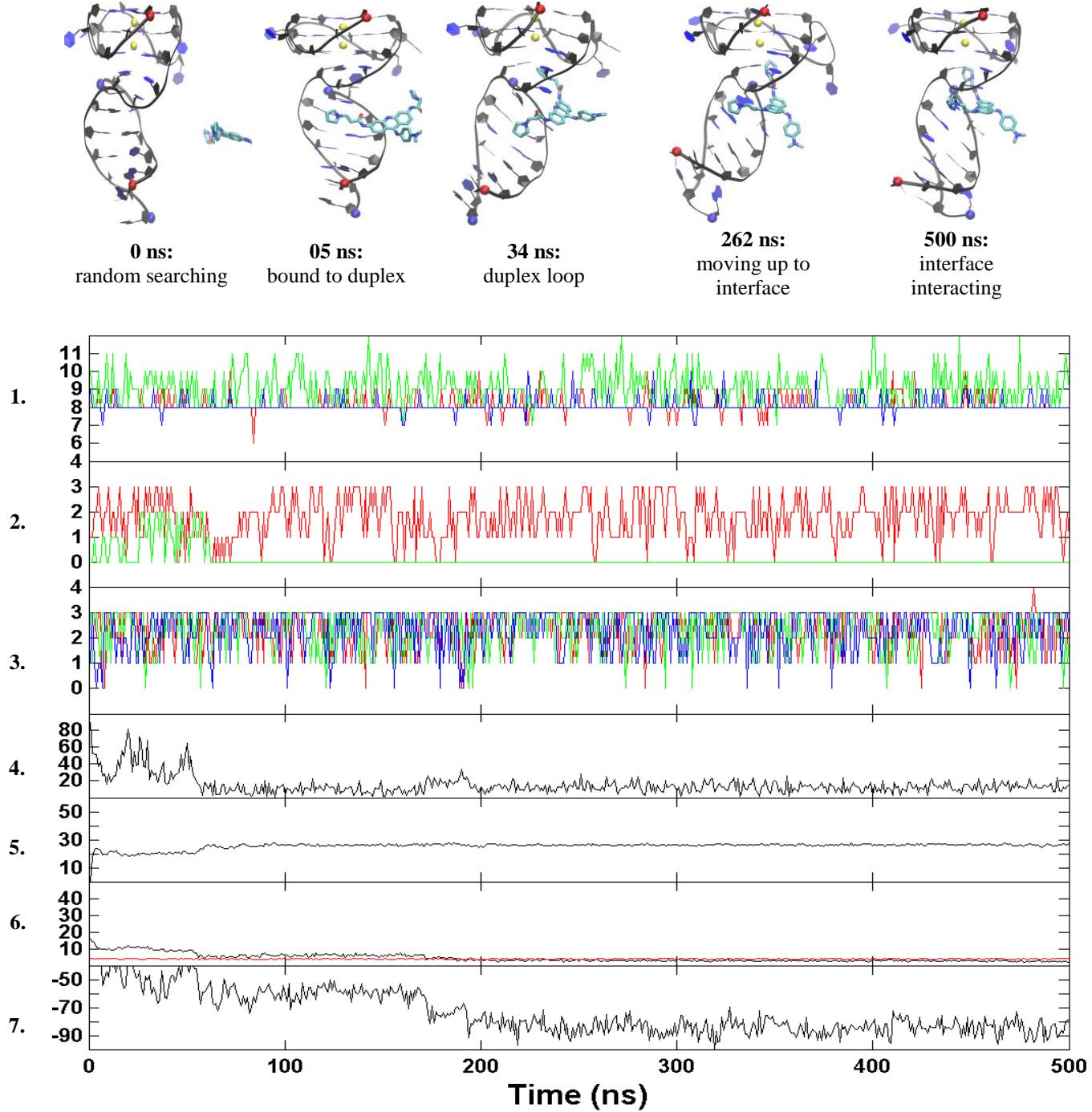


Figure S29. BRACO19, run 10, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

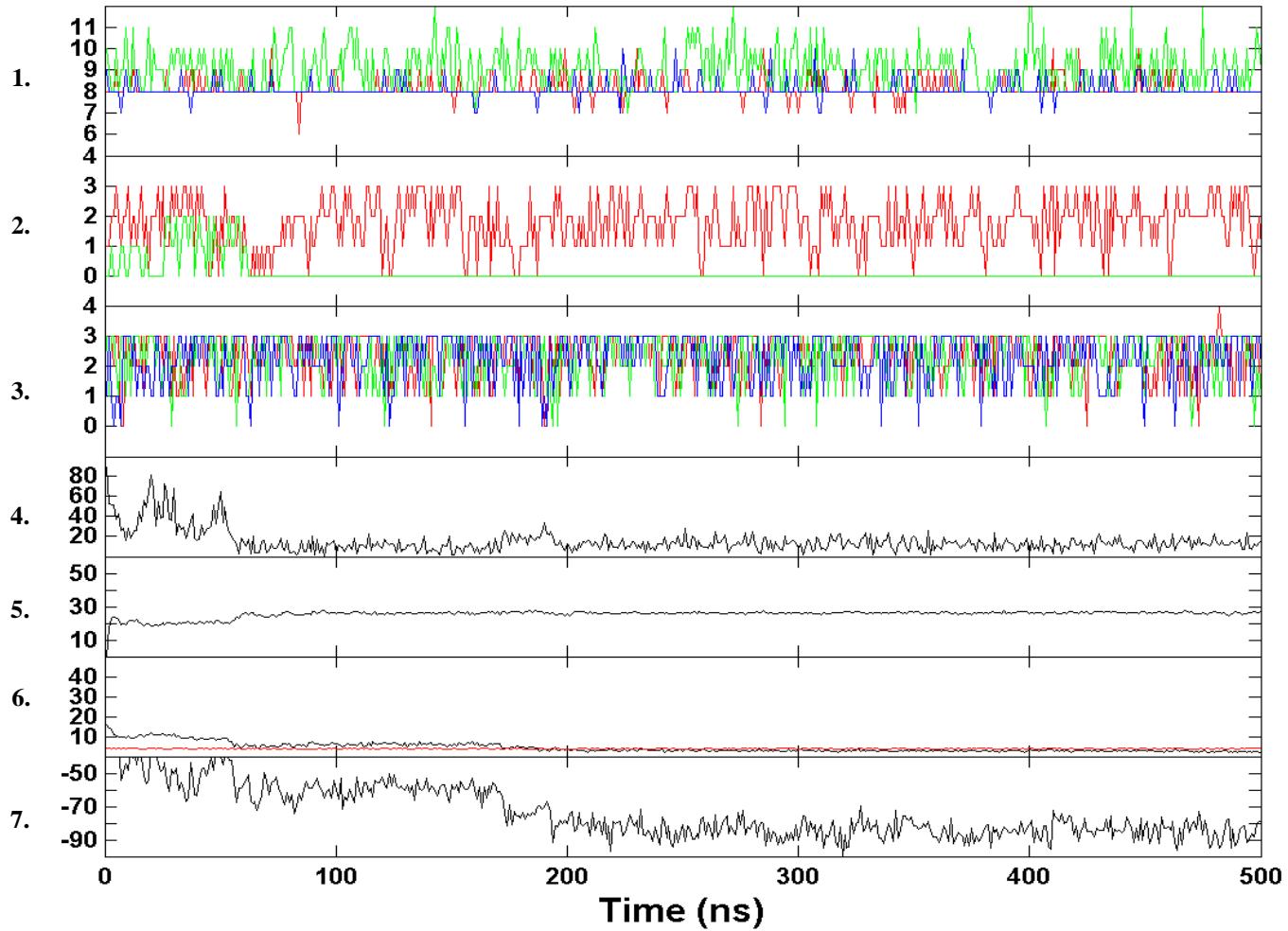
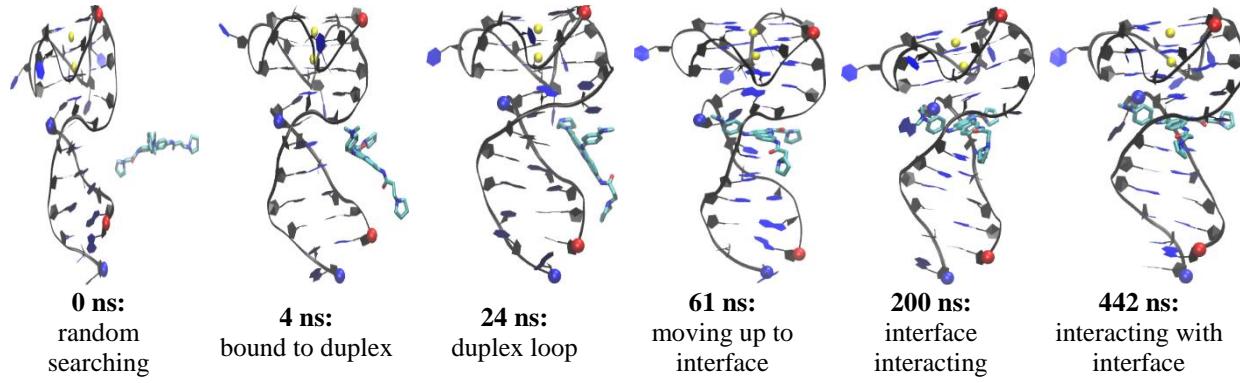


Figure S30. BRACO19, run 13, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

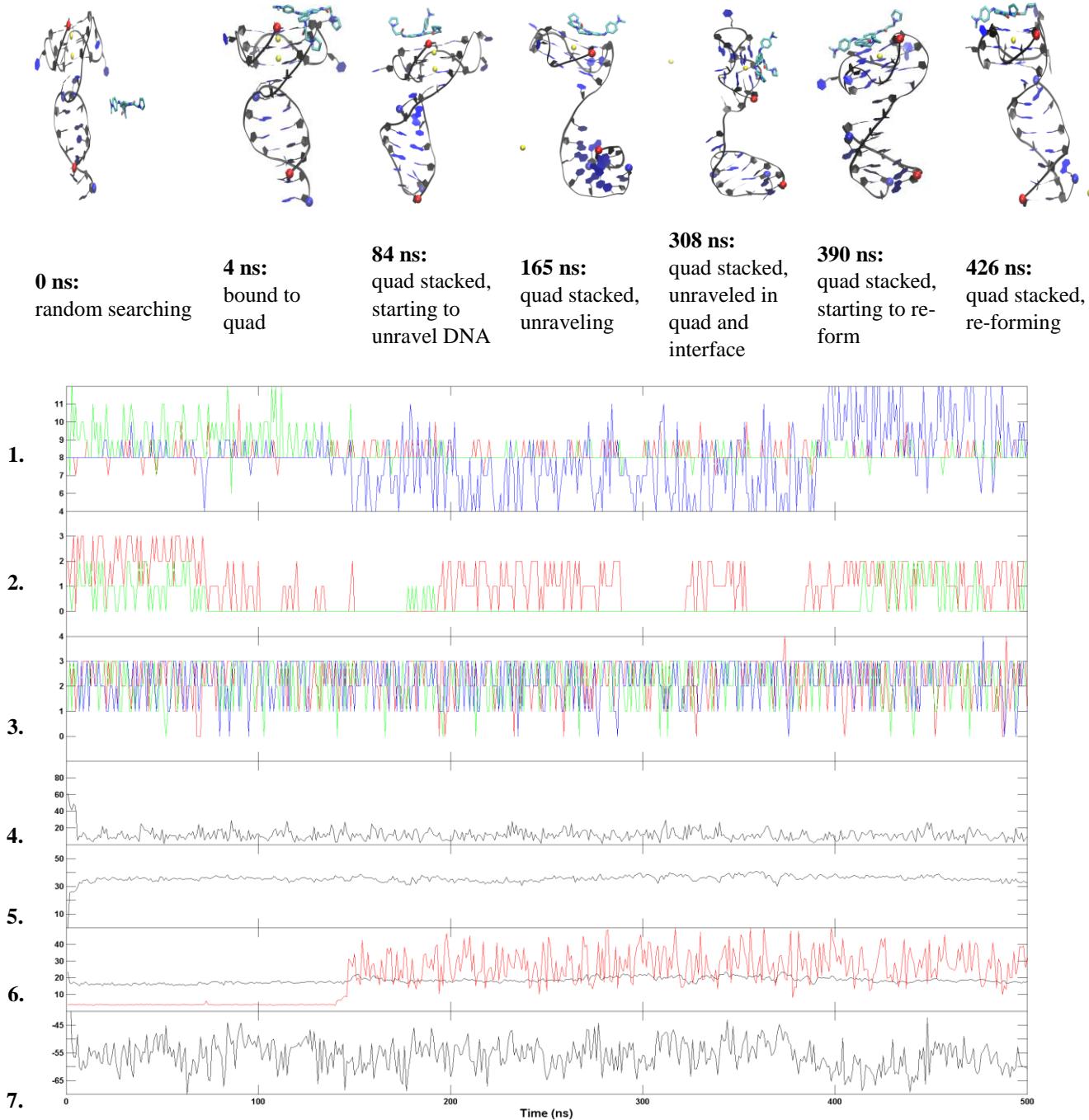


Figure S31. BRACO19, run 17, trajectory snapshots and the order parameter plot, illustrating the breaking and reforming of hydrogen- bonds (at the quadruplex (1), interface (2), and duplex(3)), drug-base dihedral angle (4), ligand(black)/DNA(red) RMSD (\AA) with reference to the final structure (5), ligand center to DNA center distance(black) and K^+ to K^+ distance(red) (6), and the MM-GBSA binding energy (ΔE in kcal/mol) (7). 5' and 3' of the DNA chain are indicated by a red and blue ball, respectively. K^+ ions are indicated by yellow balls.

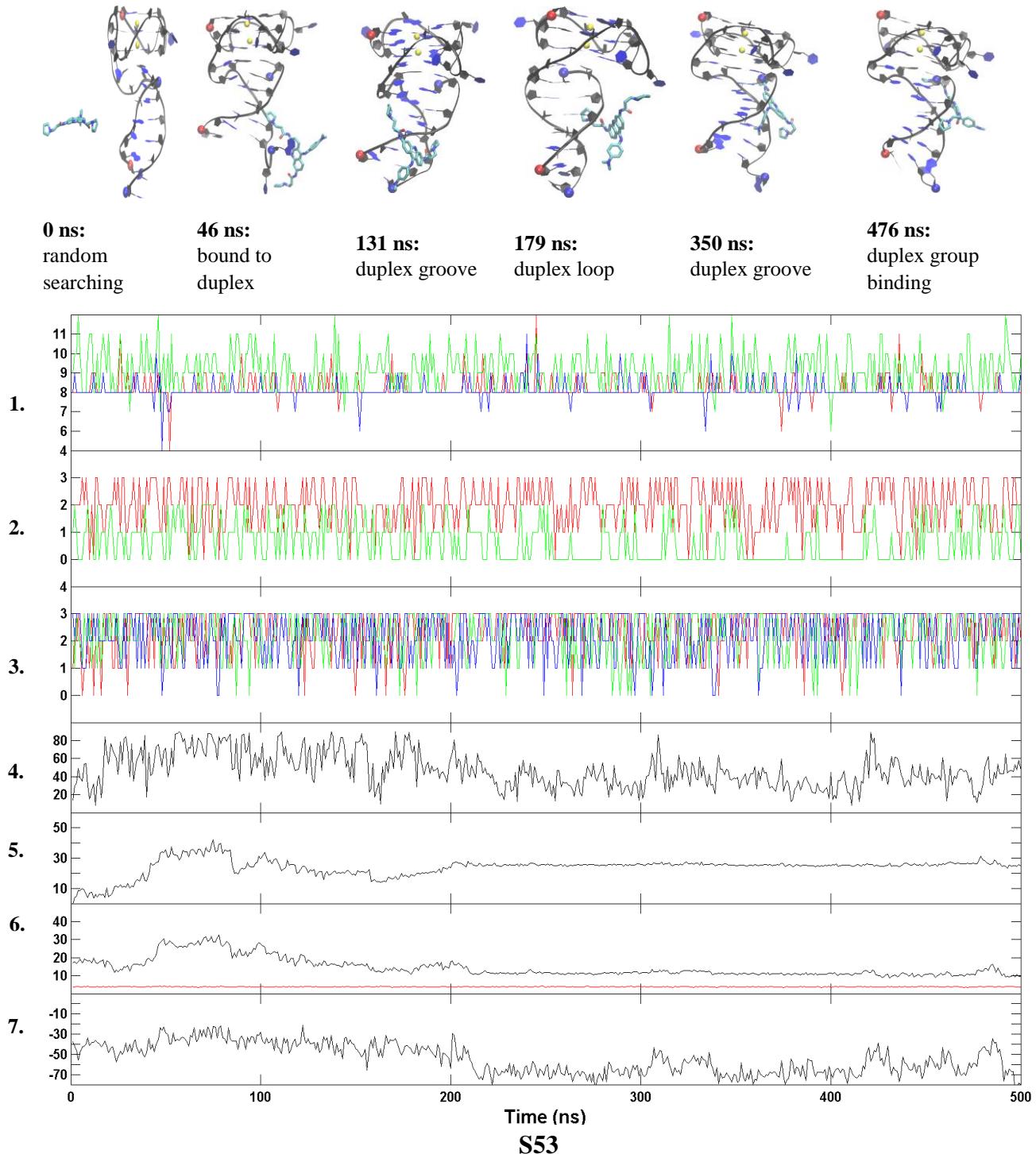
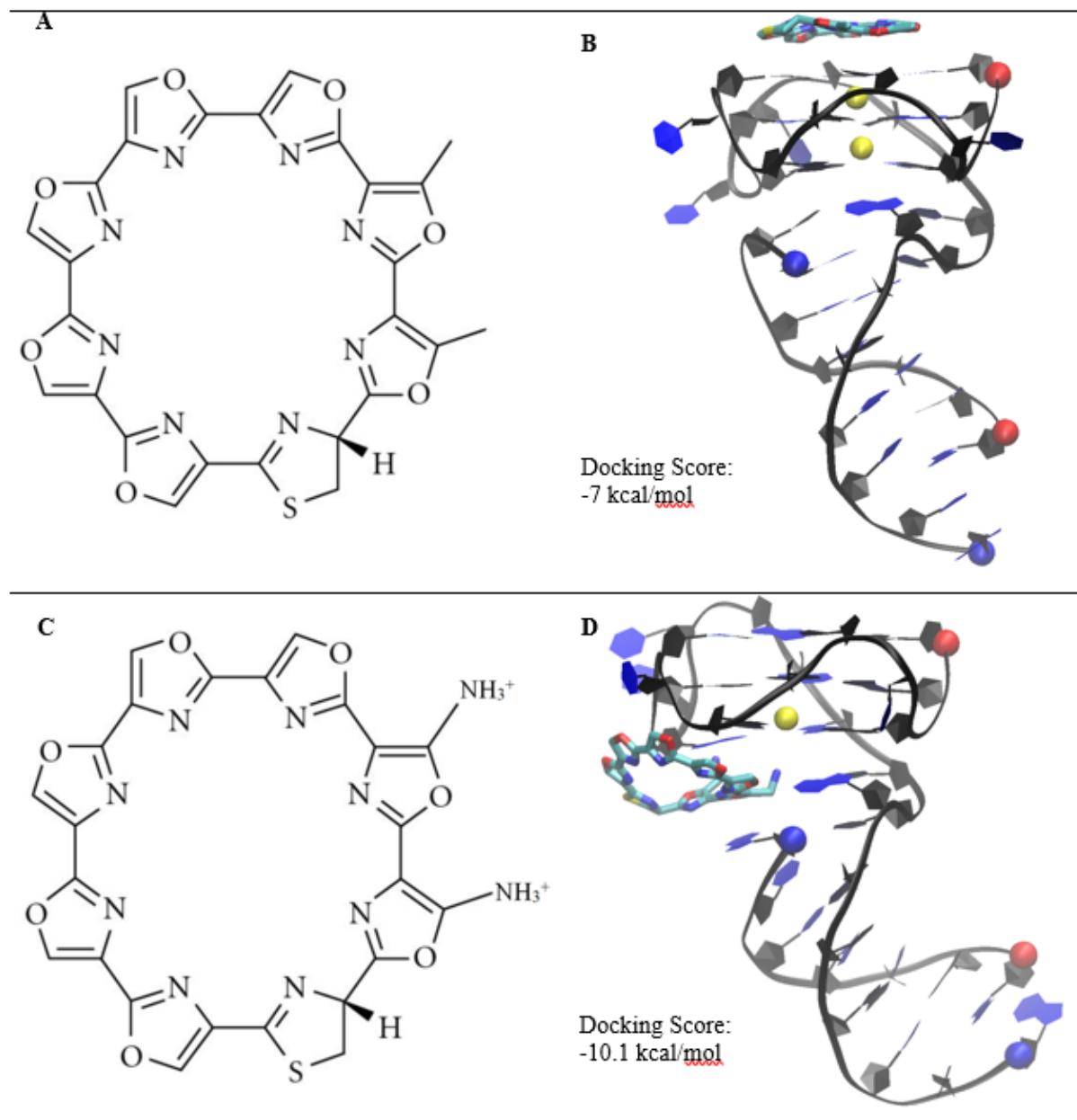
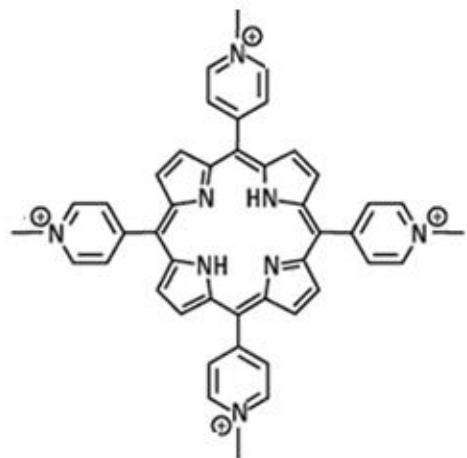
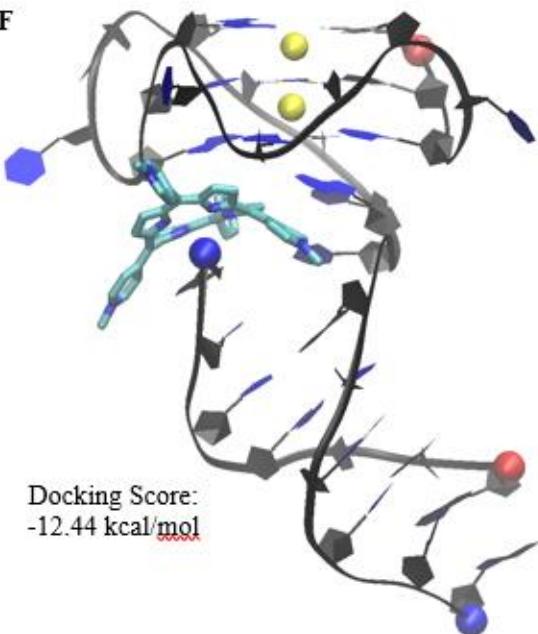


Figure S32. IFD docked results: A structure of the original Telomestatin (A), the docking pose (B), proposed Telomestatin analog (C) and the docking pose (D); A structure of the original TMPyP4 (E), the docking pose (F), proposed TMPyP4 analog (G), and the docking pose (H).



E**F**

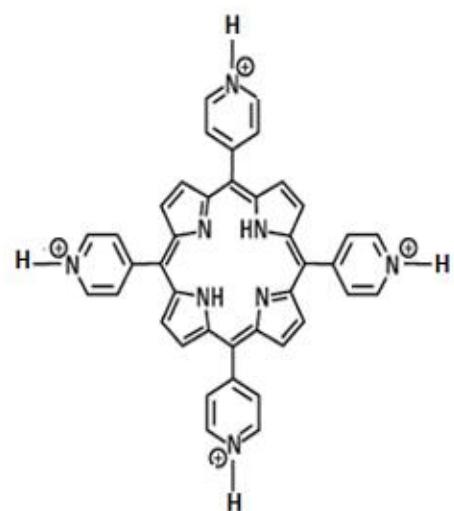
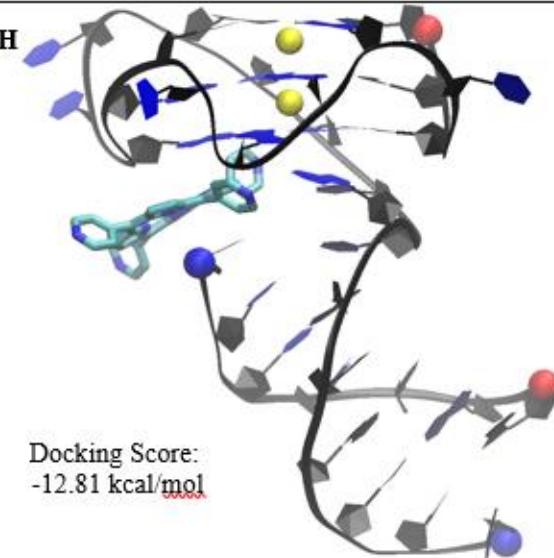
G**H**

Figure S33. AMBER GAFF2 force field of the ligands in Mol2 format.

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SMALL
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 3 C3    -2.5316  6.5930 -3.4550 C.2    1 TEL     0.0532
 4 N1    -1.9403  5.5571 -2.7937 N.2    1 TEL    -0.3885
 5 C4    -0.6532  5.7934 -2.7328 C.2    1 TEL     0.2795
 6 O1    -0.3957  6.9761 -3.3116 O.3    1 TEL    -0.1850
 7 C5    0.3202  4.8794 -2.0972 C.2    1 TEL     0.0492
 8 C6    1.6720  4.9468 -2.1590 C.2    1 TEL     0.0243
 9 O2    2.1492  3.9137 -1.4412 O.3    1 TEL    -0.1912
10 C7    1.1049  3.2471 -0.9205 C.2    1 TEL     0.2039
11 N2    0.0032  3.7961 -1.3365 N.2    1 TEL    -0.3876
12 C8    1.2113  2.0673  0.0016 C.3    1 TEL     0.1684
13 H1    1.3664  2.4475  1.0202 H     1 TEL     0.1428
14 C9    2.4448  1.2090 -0.3681 C.3    1 TEL    -0.0941
15 S1    1.7183 -0.4638 -0.1457 S.3    1 TEL    -0.1953
16 C10   0.0021 -0.0041  0.0020 C.2    1 TEL     0.3015
17 N3    -0.0156  1.2977  0.0092 N.2    1 TEL    -0.4672
18 C11   -1.1596 -0.9133  0.0903 C.2    1 TEL     0.0396
19 C12   -1.1468 -2.2127  0.4918 C.2    1 TEL     0.0015
20 O3    -2.4164 -2.6613  0.4246 O.3    1 TEL    -0.1780
21 C13   -3.1874 -1.6632 -0.0212 C.2    1 TEL     0.2685
22 N4    -2.4431 -0.5933 -0.2030 N.2    1 TEL    -0.3907
23 C14   -4.6403 -1.6861 -0.2954 C.2    1 TEL     0.0621
24 C15   -5.5406 -2.6706 -0.0733 C.2    1 TEL    -0.0065
25 O4    -6.7392 -2.2198 -0.5138 O.3    1 TEL    -0.1764
26 C16   -6.5629 -0.9903 -0.9999 C.2    1 TEL     0.2706
27 N5    -5.2996 -0.6443 -0.8538 N.2    1 TEL    -0.3902
28 C17   -7.5335 -0.0626 -1.6190 C.2    1 TEL     0.0599
29 C18   -8.8509 -0.2014 -1.8716 C.2    1 TEL    -0.0034
30 O5    -9.2668  0.9449 -2.4638 O.3    1 TEL    -0.1776
31 C19   -8.2157  1.7592 -2.5646 C.2    1 TEL     0.2715
32 N6    -7.1566  1.1662 -2.0550 N.2    1 TEL    -0.3889
33 C20   -8.1119  3.1224 -3.1301 C.2    1 TEL     0.0595
34 C21   -9.0435  3.9206 -3.6893 C.2    1 TEL    -0.0033
35 O6    -8.4207  5.0705 -4.0462 O.3    1 TEL    -0.1778
36 C22   -7.1354  4.9637 -3.7082 C.2    1 TEL     0.2718
37 N7    -6.9302  3.7901 -3.1482 N.2    1 TEL    -0.3888
38 C23   -6.0183  5.9182 -3.8748 C.2    1 TEL     0.0596
39 C24   -5.9870  7.1586 -4.4026 C.2    1 TEL    -0.0045
40 O7    -4.7062  7.5936 -4.3226 O.3    1 TEL    -0.1804
41 C25   -3.9786  6.6275 -3.7560 C.2    1 TEL     0.2790
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42 N8	-4.7589	5.6096	-3.4699	N.2	1 TEL	-0.3916
43 C26	2.4859	5.9821	-2.8915	C.3	1 TEL	-0.0757
44 H2	-1.9424	9.5835	-3.7488	H	1 TEL	0.0981
45 H3	-0.8507	9.0350	-5.0432	H	1 TEL	0.0919
46 H4	-2.5988	8.7209	-5.1606	H	1 TEL	0.1002
47 H5	3.2700	1.3797	0.3233	H	1 TEL	0.1400
48 H6	2.7537	1.3748	-1.4002	H	1 TEL	0.1181
49 H7	-0.2821	-2.7791	0.8048	H	1 TEL	0.2370
50 H8	-5.3414	-3.6342	0.3719	H	1 TEL	0.2385
51 H9	-9.4602	-1.0637	-1.6444	H	1 TEL	0.2384
52 H10	-10.0891	3.6877	-3.8270	H	1 TEL	0.2384
53 H11	-6.8251	7.7029	-4.8121	H	1 TEL	0.2383
54 H12	2.6914	6.8204	-2.2259	H	1 TEL	0.0983
55 H13	3.4265	5.5395	-3.2194	H	1 TEL	0.0915
56 H14	1.9286	6.3352	-3.7592	H	1 TEL	0.0983

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TMPyP4 (charge +4)

@<TRIPOS>MOLECULE

POH

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SMALL

No Charge or Current Charge

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1 CX3	5.1540	4.7790	-1.2200	ca	1 POH	-0.007700
2 H51	5.6840	5.0630	-2.1080	h4	1 POH	0.186325
3 C2A	-0.6640	4.2590	0.0070	cc	1 POH	-0.025124
4 H11	-1.3010	5.1180	0.0170	ha	1 POH	0.084618
5 C71	3.5040	3.4990	-0.0430	ca	1 POH	0.047749
6 C81	3.8880	4.1720	1.1130	ca	1 POH	-0.002951
7 H31	3.4260	3.9620	2.0580	ha	1 POH	0.140429
8 C91	4.8860	5.1190	1.0570	ca	1 POH	-0.007700
9 H41	5.2100	5.6540	1.9280	h4	1 POH	0.186325
10 CXN	6.5790	6.4350	-0.1400	c3	1 POH	-0.008606
11 H811	6.7180	6.8450	0.8460	h1	1 POH	0.106092
12 H821	6.2870	7.2180	-0.8230	h1	1 POH	0.106092
13 H831	7.4930	5.9650	-0.4710	h1	1 POH	0.106092
14 C3A	0.6640	4.2590	-0.0070	cc	1 POH	-0.025555
15 H21	1.3010	5.1180	-0.0170	ha	1 POH	0.088596
16 C4A	1.1320	2.8690	-0.0070	cd	1 POH	-0.006562
17 C1A	-1.1320	2.8690	0.0070	cd	1 POH	-0.006343
18 CXD	4.1680	3.8250	-1.2280	ca	1 POH	-0.002951
19 H61	3.9170	3.3450	-2.1540	ha	1 POH	0.140429
20 NXT	5.5010	5.4110	-0.0910	na	1 POH	0.010373
21 NA	0.0000	2.1000	0.0000	na	1 POH	0.012242
22 H71	0.0000	1.1050	0.0000	hn	1 POH	0.020707
23 NB	2.0600	0.0300	-0.0180	nc	1 POH	-0.018987
24 NC	0.0000	-2.0900	0.0000	na	1 POH	-0.014127
25 H73	0.0000	-1.0940	0.0000	hn	1 POH	0.066398
26 ND	-2.0600	0.0300	0.0180	nc	1 POH	-0.023026
27 CHB	2.4230	2.4510	-0.0210	cf	1 POH	-0.047656
28 C1B	2.8500	1.0620	-0.0140	cc	1 POH	-0.027173
29 CX4	5.0220	-4.9580	-1.0510	cc	1 POH	-0.007699
30 H52	5.4730	-5.3700	-1.9310	h4	1 POH	0.186325
31 C2B	4.2670	0.6700	0.0220	cc	1 POH	-0.046218
32 H12	5.1110	1.3260	0.0430	ha	1 POH	0.068051
33 C72	3.5180	-3.4650	0.0570	cc	1 POH	0.047749
34 C82	3.9550	-4.0020	1.2680	cc	1 POH	-0.002951
35 H32	3.5620	-3.6570	2.2040	ha	1 POH	0.140429
36 C92	4.9080	-4.9890	1.2650	cd	1 POH	-0.007699
37 H42	5.2780	-5.4300	2.1710	h4	1 POH	0.186325
38 CXO	6.4640	-6.5180	0.1790	c3	1 POH	-0.008606
39 H812	6.0770	-7.3520	0.7440	h1	1 POH	0.106091
40 H822	7.3490	-6.1190	0.6510	h1	1 POH	0.106091
41 H832	6.6960	-6.8360	-0.8230	h1	1 POH	0.106091
42 C3B	4.2820	-0.6600	0.0370	cd	1 POH	-0.047477
43 H22	5.1420	-1.2950	0.0680	ha	1 POH	0.098118

44 C4B	2.8830	-1.0930	0.0120 cd	1 POH	-0.026907
45 CXE	4.0700	-3.9660	-1.1160 cd	1 POH	-0.002951
46 H62	3.7700	-3.5950	-2.0770 ha	1 POH	0.140429
47 NXU	5.4260	-5.4540	0.1210 na	1 POH	0.010373
48 CHC	2.4700	-2.3830	0.0240 cf	1 POH	-0.028644
49 C1C	1.1120	-2.8680	0.0120 cd	1 POH	-0.038967
50 CX5	-4.9080	-4.9890	-1.2650 ca	1 POH	-0.007699
51 H53	-5.2780	-5.4300	-2.1710 h4	1 POH	0.186325
52 C2C	0.6940	-4.1930	0.0070 cc	1 POH	-0.085258
53 H13	1.3210	-5.0590	0.0120 ha	1 POH	0.103774
54 C73	-3.5180	-3.4650	-0.0570 ca	1 POH	0.047749
55 C83	-4.0700	-3.9660	1.1160 ca	1 POH	-0.002951
56 H33	-3.7700	-3.5950	2.0770 ha	1 POH	0.140429
57 C93	-5.0220	-4.9580	1.0510 ca	1 POH	-0.007699
58 H43	-5.4730	-5.3700	1.9310 h4	1 POH	0.186325
59 CXP	-6.4640	-6.5180	-0.1790 c3	1 POH	-0.008606
60 H813	-6.6960	-6.8360	0.8230 h1	1 POH	0.106091
61 H823	-6.0770	-7.3520	-0.7440 h1	1 POH	0.106091
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63 C3C	-0.6940	-4.1930	-0.0070 cc	1 POH	-0.084183
64 H23	-1.3210	-5.0590	-0.0120 ha	1 POH	0.100100
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66 CXF	-3.9550	-4.0020	-1.2680 ca	1 POH	-0.002951
67 H63	-3.5620	-3.6570	-2.2040 ha	1 POH	0.140429
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71 CX6	-4.8860	5.1190	-1.0570 cd	1 POH	-0.007699
72 H54	-5.2100	5.6540	-1.9280 h4	1 POH	0.186325
73 C2D	-4.2820	-0.6600	-0.0370 cc	1 POH	-0.048886
74 H14	-5.1420	-1.2950	-0.0680 ha	1 POH	0.098104
75 C74	-3.5040	3.4990	0.0430 cc	1 POH	0.047749
76 C84	-4.1680	3.8250	1.2280 cc	1 POH	-0.002951
77 H34	-3.9170	3.3450	2.1540 ha	1 POH	0.140429
78 C94	-5.1540	4.7790	1.2200 cd	1 POH	-0.007699
79 H44	-5.6840	5.0630	2.1080 h4	1 POH	0.186325
80 CXQ	-6.5790	6.4350	0.1400 c3	1 POH	-0.008606
81 H814	-6.2870	7.2180	0.8230 h1	1 POH	0.106091
82 H824	-7.4930	5.9650	0.4710 h1	1 POH	0.106091
83 H834	-6.7180	6.8450	-0.8460 h1	1 POH	0.106091
84 C3D	-4.2670	0.6700	-0.0220 cd	1 POH	-0.047915
85 H24	-5.1110	1.3260	-0.0430 ha	1 POH	0.069437
86 C4D	-2.8500	1.0620	0.0140 cd	1 POH	-0.025977
87 CXG	-3.8880	4.1720	-1.1130 cc	1 POH	-0.002951
88 H64	-3.4260	3.9620	-2.0580 ha	1 POH	0.140429
89 CHA	-2.4230	2.4510	0.0210 cf	1 POH	-0.045275
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@<TRIPOS>SUBSTRUCTURE

1 POH 1 TEMP 0 **** * ROOT

BSU6037 (+2)

@<TRIPOS>MOLECULE

BSU

69 73 1 0 0

SMALL

rc

@<TRIPOS>ATOM

1 O1	-4.7600	0.7650	-0.2000 o	1 BSU	-0.482839
2 C1	-5.5760	-0.1280	-0.2480 c	1 BSU	0.484728
3 C2	-7.0630	0.2070	-0.2930 c3	1 BSU	-0.058780
4 H1	-7.6120	-0.5270	-0.8710 hc	1 BSU	0.067648
5 H2	-7.4530	0.1550	0.7190 hc	1 BSU	0.067648
6 C3	-7.3340	1.5750	-0.9180 c3	1 BSU	-0.084247
7 H3	-6.9620	1.6020	-1.9330 hx	1 BSU	0.106335
8 H4	-8.3950	1.7810	-0.9360 hx	1 BSU	0.106335
9 N1	-6.6680	2.6930	-0.1900 n4	1 BSU	0.044582
10 H34	-5.6960	2.4060	-0.1280 hn	1 BSU	0.235503
11 C4	-7.1610	2.9530	1.2130 c3	1 BSU	-0.045295
12 H5	-8.1930	2.6400	1.2670 hx	1 BSU	0.091457
13 H6	-6.5750	2.3480	1.8890 hx	1 BSU	0.091457
14 C5	-6.9960	4.4690	1.4370 c3	1 BSU	-0.049412
15 H7	-7.9690	4.9290	1.5520 hc	1 BSU	0.065879
16 H8	-6.4290	4.6770	2.3340 hc	1 BSU	0.065879
17 C6	-6.2960	4.9940	0.1730 c3	1 BSU	-0.014718
18 H9	-6.5820	6.0070	-0.0740 hc	1 BSU	0.056351
19 H10	-5.2180	4.9720	0.2860 hc	1 BSU	0.056351
20 C7	-6.7250	4.0090	-0.9030 c3	1 BSU	-0.037789
21 H11	-6.0860	3.9690	-1.7730 hx	1 BSU	0.087642
22 H12	-7.7490	4.1690	-1.2150 hx	1 BSU	0.087642
23 N2	-5.2880	-1.4350	-0.2350 n	1 BSU	-0.338422
24 H13	-6.0640	-2.0570	-0.2860 hn	1 BSU	0.291326
25 C8	-4.0280	-2.0790	-0.1240 ca	1 BSU	0.027572
26 C9	-4.1070	-3.5070	0.0140 ca	1 BSU	-0.183473
27 H14	-5.0700	-3.9850	0.0350 ha	1 BSU	0.167471
28 C10	-2.9870	-4.2430	0.1200 ca	1 BSU	-0.216878
29 H15	-3.0480	-5.3110	0.2230 ha	1 BSU	0.185849
30 C11	-1.7000	-3.6190	0.0970 ca	1 BSU	0.019035
31 C12	-0.5120	-4.3250	0.1990 ca	1 BSU	-0.118265
32 H16	-0.5270	-5.3960	0.3040 ha	1 BSU	0.160961
33 C13	0.6940	-3.6460	0.1630 ca	1 BSU	0.041610
34 C14	1.9640	-4.2990	0.2580 ca	1 BSU	-0.224115
35 H17	1.9950	-5.3680	0.3660 ha	1 BSU	0.183539
36 C15	3.1030	-3.5890	0.2130 ca	1 BSU	-0.176207
37 H18	4.0530	-4.0890	0.2840 ha	1 BSU	0.162225
38 C16	3.0690	-2.1580	0.0680 ca	1 BSU	0.038389
39 N3	4.3440	-1.5460	0.0300 n	1 BSU	-0.403529
40 H19	5.1090	-2.1780	0.1070 hn	1 BSU	0.298499
41 C17	4.6520	-0.2390	-0.1040 c	1 BSU	0.573260
42 O2	3.8700	0.6610	-0.2090 o	1 BSU	-0.504283
43 C18	6.1560	0.0480	-0.1120 c3	1 BSU	0.006734
44 H20	6.5930	-0.3200	0.8110 hc	1 BSU	0.020202

45 H21	6.6180	-0.4990	-0.9310 hc	1 BSU	0.020202
46 C19	6.3710	1.5490	-0.2720 c3	1 BSU	-0.147715
47 H22	5.8890	1.9050	-1.1690 hx	1 BSU	0.121798
48 H23	5.9660	2.0960	0.5650 hx	1 BSU	0.121798
49 N4	7.8220	1.9080	-0.3770 n4	1 BSU	0.007785
50 H35	8.2170	1.3700	-1.1330 hn	1 BSU	0.293757
51 C20	8.0650	3.3550	-0.7090 c3	1 BSU	-0.086699
52 H24	7.7430	3.5460	-1.7220 hx	1 BSU	0.121908
53 H25	7.4650	3.9390	-0.0250 hx	1 BSU	0.121908
54 C21	9.5550	3.5180	-0.4550 c3	1 BSU	-0.017603
55 H26	10.1210	3.1540	-1.3070 hc	1 BSU	0.060262
56 H27	9.8200	4.5560	-0.3100 hc	1 BSU	0.060262
57 C22	9.8200	2.6560	0.7950 c3	1 BSU	-0.046537
58 H28	10.7770	2.1580	0.7430 hc	1 BSU	0.078015
59 H29	9.8170	3.2620	1.6910 hc	1 BSU	0.078015
60 C23	8.6600	1.6410	0.8540 c3	1 BSU	-0.171611
61 H30	8.0190	1.7990	1.7090 hx	1 BSU	0.148125
62 H31	8.9760	0.6100	0.8400 hx	1 BSU	0.148125
63 C24	1.8930	-1.4970	-0.0230 ca	1 BSU	-0.084367
64 H32	1.8380	-0.4360	-0.1310 ha	1 BSU	0.122242
65 C25	0.6590	-2.2300	0.0220 ca	1 BSU	0.304403
66 N5	-0.4730	-1.5490	-0.0730 nb	1 BSU	-0.554121
67 C26	-1.6230	-2.2060	-0.0390 ca	1 BSU	0.318340
68 C27	-2.8360	-1.4440	-0.1500 ca	1 BSU	-0.073941
69 H33	-2.7480	-0.3850	-0.2530 ha	1 BSU	0.101795

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@<TRIPOS>SUBSTRUCTURE

1 BSU 1 TEMP 0 **** 0 ROOT

BRACO19 (Charge +3)

@<TRIPOS>MOLECULE

BRA

90 95 1 0 0

SMALL

Current Charge

@<TRIPOS>ATOM

1 C40	7.9610	-6.2860	0.7000	c3	1 BRA	0.087538
2 H402	7.3030	-6.8400	0.0440	hx	1 BRA	0.059896
3 H403	7.6520	-6.4280	1.7250	hx	1 BRA	0.059896
4 C41	9.4290	-6.5640	0.4170	c3	1 BRA	-0.112692
5 H412	10.0400	-6.2250	1.2460	hc	1 BRA	0.090060
6 H413	9.6120	-7.6220	0.2920	hc	1 BRA	0.090060
7 C42	9.7280	-5.7550	-0.8600	c3	1 BRA	-0.212900
8 H422	10.7190	-5.3260	-0.8400	hc	1 BRA	0.106253
9 H423	9.6630	-6.3800	-1.7410	hc	1 BRA	0.106253
10 C43	8.6430	-4.6600	-0.9240	c3	1 BRA	0.073604
11 H432	9.0330	-3.6550	-0.9490	hx	1 BRA	0.089004
12 H433	7.9700	-4.7970	-1.7580	hx	1 BRA	0.089004
13 N39	7.8190	-4.8290	0.3350	n4	1 BRA	0.041483
14 H39	8.2770	-4.3080	1.0680	hn	1 BRA	0.234943
15 C38	6.3980	-4.3670	0.2600	c3	1 BRA	0.151616
16 H382	5.9300	-4.9050	-0.5500	hx	1 BRA	0.056508
17 H383	5.9170	-4.6630	1.1800	hx	1 BRA	0.056508
18 C37	6.2850	-2.8570	0.0610	c3	1 BRA	-0.051039
19 H372	6.7200	-2.5470	-0.8840	hc	1 BRA	0.019218
20 H373	6.8080	-2.3210	0.8490	hc	1 BRA	0.019218
21 C36	4.8130	-2.4500	0.0820	c	1 BRA	0.077607
22 O52	3.9490	-3.2600	0.2300	o	1 BRA	-0.318082
23 N17	4.6040	-1.1110	-0.0820	n	1 BRA	0.021983
24 H17	5.4140	-0.5430	-0.1970	hn	1 BRA	0.274090
25 C3	3.3930	-0.4140	-0.1070	cc	1 BRA	-0.047222
26 C4	2.1610	-1.0000	0.0320	cc	1 BRA	-0.028874
27 H4	2.0650	-2.0560	0.1640	ha	1 BRA	0.058651
28 C2	3.4860	0.9840	-0.2980	cc	1 BRA	-0.108732
29 H2	4.4470	1.4460	-0.4280	ha	1 BRA	0.093141
30 C1	2.3690	1.7530	-0.3200	cd	1 BRA	-0.031756
31 H1	2.4860	2.8020	-0.4730	ha	1 BRA	0.107640
32 C6	1.0710	1.1960	-0.1650	cd	1 BRA	0.016672
33 C10	-0.1620	1.9530	-0.1570	cc	1 BRA	0.025953
34 N19	-0.2420	3.2660	-0.1120	nh	1 BRA	-0.010247
35 H19	-1.1650	3.6330	-0.0640	hn	1 BRA	0.209058
36 C28	0.7660	4.2930	-0.0190	ca	1 BRA	-0.061182
37 C29	1.1510	4.9930	-1.1500	ca	1 BRA	-0.078570
38 H29	0.7440	4.7310	-2.1110	ha	1 BRA	0.117670
39 C24	2.0560	6.0280	-1.0610	ca	1 BRA	-0.077042
40 H24	2.3230	6.5470	-1.9590	ha	1 BRA	0.097661
41 C25	2.6040	6.4150	0.1790	ca	1 BRA	-0.073543
42 N15	3.5020	7.4340	0.2740	nh	1 BRA	-0.070436
43 C16	3.9440	7.8960	1.5780	c3	1 BRA	-0.023951

44 H161	4.6470	8.7030	1.4470 h1	1 BRA	0.059635
45 H162	4.4500	7.1070	2.1230 h1	1 BRA	0.059635
46 H163	3.1190	8.2620	2.1820 h1	1 BRA	0.059635
47 C18	3.8190	8.2360	-0.8960 c3	1 BRA	-0.023951
48 H181	4.5460	8.9840	-0.6240 h1	1 BRA	0.059635
49 H182	2.9440	8.7440	-1.2910 h1	1 BRA	0.059635
50 H183	4.2530	7.6280	-1.6820 h1	1 BRA	0.059635
51 C26	2.1810	5.6970	1.3170 ca	1 BRA	-0.077042
52 H26	2.5460	5.9560	2.2900 ha	1 BRA	0.097661
53 C27	1.2750	4.6650	1.2140 ca	1 BRA	-0.078570
54 H27	0.9630	4.1480	2.1050 ha	1 BRA	0.117670
55 C5	1.0070	-0.2010	-0.0130 cd	1 BRA	-0.016707
56 N7	-0.1970	-0.8260	0.1000 na	1 BRA	-0.038303
57 H90	-0.1990	-1.8150	0.2200 hn	1 BRA	0.296107
58 C8	-1.3900	-0.1830	-0.0250 ca	1 BRA	-0.035004
59 C11	-2.5780	-0.9230	0.0100 ca	1 BRA	-0.107796
60 H11	-2.5220	-1.9890	0.1500 ha	1 BRA	0.071170
61 C9	-1.4110	1.2050	-0.1850 ca	1 BRA	-0.009844
62 C14	-2.6800	1.8040	-0.3590 ca	1 BRA	-0.055215
63 H14	-2.7720	2.8570	-0.5410 ha	1 BRA	0.138532
64 C13	-3.8420	1.0970	-0.3420 ca	1 BRA	-0.031591
65 H13	-4.7750	1.5940	-0.4860 ha	1 BRA	0.107484
66 C12	-3.7960	-0.3010	-0.1390 ca	1 BRA	-0.047363
67 N21	-4.9440	-1.0990	-0.0950 n	1 BRA	0.021983
68 H21	-4.7780	-2.0720	0.0440 hn	1 BRA	0.274090
69 C44	-6.2520	-0.7130	-0.2070 c	1 BRA	0.077607
70 O53	-6.6190	0.4090	-0.3740 o	1 BRA	-0.318082
71 C45	-7.2630	-1.8530	-0.0990 c3	1 BRA	-0.051039
72 H452	-7.0450	-2.5980	-0.8610 hc	1 BRA	0.019218
73 H453	-7.1480	-2.3340	0.8670 hc	1 BRA	0.019218
74 C46	-8.6690	-1.2800	-0.2780 c3	1 BRA	0.151616
75 H462	-8.7490	-0.7730	-1.2270 hx	1 BRA	0.056508
76 H463	-8.9010	-0.5690	0.4990 hx	1 BRA	0.056508
77 N47	-9.7330	-2.3300	-0.2480 n4	1 BRA	0.041483
78 H47	-9.5090	-3.0230	-0.9470 hn	1 BRA	0.234943
79 C48	-11.1040	-1.8050	-0.5980 c3	1 BRA	0.087539
80 H482	-11.1240	-1.5340	-1.6440 hx	1 BRA	0.059896
81 H483	-11.2650	-0.9220	0.0060 hx	1 BRA	0.059896
82 C49	-12.0180	-2.9530	-0.2020 c3	1 BRA	-0.112692
83 H492	-13.0360	-2.6160	-0.0640 hc	1 BRA	0.090060
84 H493	-12.0290	-3.7080	-0.9800 hc	1 BRA	0.090060
85 C50	-11.3940	-3.5000	1.0960 c3	1 BRA	-0.212900
86 H502	-11.8810	-3.0830	1.9670 hc	1 BRA	0.106253
87 H503	-11.4800	-4.5760	1.1600 hc	1 BRA	0.106253
88 C51	-9.9170	-3.0560	1.0680 c3	1 BRA	0.073604
89 H512	-9.2110	-3.8710	1.1150 hx	1 BRA	0.089004
90 H513	-9.6870	-2.3470	1.8510 hx	1 BRA	0.089004

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@<TRIPOS>SUBSTRUCTURE

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